EXAMINING MEAN-FIELD APPROXIMATIONS AND BOGOLIUBOV-DE GENNES (BDG) EQUATIONS FOR TOPOLOGICAL QUANTUM COMPUTING - SOME CONSIDERATIONS ON THE CONCEPTUAL BASIS OF MAJORANA ZERO MODES IN P+IP SUPERCONDUCTORS

BY

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DISSERTATION

Submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy in Physics
in the Graduate College of the
University of Illinois at Urbana-Champaign, 2017

Urbana, Illinois

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Abstract

The current theoretical framework for studying Majorana zero modes (MZM) in superconductors and its application for topological quantum computing is based on mean-field approximations and is derived from solutions to BdG equations. In this framework, particle number conservation is broken and non-interacting fermion Hamiltonian is used to describe physics of interest. We argue that these features in the current framework may make it insufficient for studying topological properties of MZM pertinent to quantum computing. After reviewing the current theory with an emphasis on its potential problems, we investigate physics beyond the BdG equations in a toy model and find evidence for the non-trivial role of particle number conservation in Berry phase of transporting a bound quasiparticle around a vortex in a s-wave superconductor. We then study the effect of particle number conservation and superconducting condensate on braiding MZM in vortices in chiral p-wave superconductors and find that they may have non-negligible effect on properties of MZM, suggesting the need for further study on the theoretical basis of this intriguing subject.

To my family.

Acknowledgments

I didn't intend to make this sound like Oscar award speech. I didn't win anything. But I couldn't help being emotional when I actually started writing this part. There are so many people I am indebted to. Transferred from another major which bears little relevance to modern physics, it would be impossible for this to happen without the help and encouragement of many great people both in Physics Department and elsewhere. I want to especially thank Professor John Stack for his kindness, encouragement and help, in particular when I was applying for graduate program in physics while he was associate Dean in charge of enrolling new graduate students. I want to thank Professor Xue-xiong Shan, Professor Jim Eckstein, Professor Lance Cooper and Professor Igor G. Nikolaev for their support in my application for graduate studies in physics. I want to thank Professor Paul Goldbart whose quantum mechanics class I was auditing from the middle of the semester when I decided to apply for physics. I was then even given the chance to take part in the final exam with a final grade. This was incredible experience for me. I want to thank Professor Russ Giannetta for his patient help in his E&M class which I took before I became a graduate student in physics. I want to thank Professor Mike Stone for his invaluable help during the time we wrote a paper together and during the early stage of my PhD work presented here. I want to thank Professor Jim Eckstein and his student Stephanie Law for insightful discussions that motivated my work with Mike. I also want to thank our great physics staff for their kind help, in particular Wendy Wimmer, Mel Schweighart, Becky McDuffee and Janice Benner. I want to thank my former officemate Minh Pham whom we shared many relaxed moments.

I want to thank my advisor Professor Tony Leggett to whom I owe the most. His attitude towards people and towards doing physics impresses me the most. I was given an opportunity to talk to him about research even before I became a physics student. I was also fortunate enough to be accepted as his student, given my non-physics background. I greatly appreciate his endless patience on my complete ignorance especially during my early years as his student. This thesis wouldn't be possible without his invaluable guidance and enormous effort. I feel ashamed that I almost only did the rather trivial part of the work.

Finally, I want to thank all my family members for their endless support, patience and love. Without them, I wouldn't be able to persist in pursuing my PhD in physics. I dedicate this thesis to them, and in particular to my beloved father in heaven.

This work was supported by the National Science Foundation through grant NSF-DMR-09-06921.

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Chapter 1

Introduction

The prediction of Majorana zero modes (MZM) in superconductors and its potential application to topological quantum computing has raised a lot of excitement and stimulated intensive research effort in both theoretical proposals for creating it in a wide variety of systems and experimental search for its signatures (for a previous review, see [1] and there are many more work more recently, for example, [2], [3]). So far, no smoking-gun experimental evidence is established to demonstrate its non-Abelian topological properties (available experiments focus on zero energy feature of MZM, for example, [4], [5]). In the meanwhile, little attention is being paid to the justification of theoretical framework used to study the Majorana zero mode. However, special caution is very much needed in regard to this subject as it lies on the interface of traditional condensed matter physics and quantum information science. The current theoretical framework is based on the mean-field approximations and Bogoliubov-de Dennes (BdG) equations which are suitable for calculating quantities that are averaged in some ways. Particle number conservation is usually unimportant, instead only average particle number is fixed. Neither is the explicit knowledge of many-body wave functions required. This suffices for most purposes. On the other hand, for purposes of quantum information processing and quantum computation, precise control of quantum states is usually crucial and quantum decoherence needs to be controlled with great care. From this perspective, there is no a priori justification to assume that the BdG equations can be straightforwardly applied for studying subtle topological properties pertinent to quantum information and quantum computing, such as non-local quantum entanglement exhibited by Majorana zero mode.

The BdG equations are set of equations for quasiparticle wave functions and the corresponding low energy spectrum. Operated at the mean-field level, the BdG equations connects even particle number parity many-body energy ground states with odd particle number parity excited eigenstates by adding/subtracting a single quasiparticle whose wave function is given by solutions to the BdG equations. The ground state is vacuum to all positive-energy quasiparticles which are non-interacting fermions obeying Fermi statistics. At defects such as vortices in superconductors with chiral p-wave pairing, solving the BdG equations yields localized zero-energy solutions. These zero-energy quasiparticles suggest not only ground state degeneracy, but highly intricate long range quantum entanglement in them which holds the key to the topological quantum computing (for a review on topological quantum computing in condensed matter systems, see [6]). The long range entanglement is deduced from the particle-hole symmetry of the BdG solutions as a consequence of unphysically breaking particle-number conservation that is the usual mathematical treatment to simplify calculations in superconductors. The particle-hole symmetry suggests that zero-energy solutions of the BdG equations have to be self-adjoint (up to overall phase factor), hence the name Majorana zero modes. Since the actual physical degrees of freedom are made of complex Dirac fermions, two Majorana zero modes combine to make one degree of freedom. So each zero-energy Dirac quasiparticle can be regarded as split into two localized Majorana zero modes and there's long range quantum entanglement between Majorana zero modes. Consequently, degenerate ground states are locally indistinguishable and these Majorana zero modes obey non-Abelian statistics. Therefore, braiding these Majorana zero modes induces unitary evolution within ground state subspace [7] which can be used to construct qubits that are topologically protected from environment decoherence [8], [9].

There are, however, loopholes in deriving from the BdG equations properties of Majorana zero modes. As the BdG equations explicitly break particle-number conservation, corresponding quasiparticles, being superpositions of particle and hole, do not conserve particle number. As a result, the corresponding energy eigenstates are not quantum states with fixed particle number, but rather are coherent superposition of different particle number with the same particle-number parity, which do not correspond to physical states that form qubits in condensed matter systems whose underlying low energy many-body eigen-states always have fixed fermion number. It is thus not immediately clear whether properties exhibited by such states as superposition of different particle number is physically relevant to the actual states of interest with fixed particle number. Although in traditional condensed matter settings, physical quantities of interest are insensitive to particle number conservation as they are averaged over macroscopic number of particles, quantities relevant to quantum information and computing application such as Berry's phase are much more subtle and may depend on many-body wave functions in delicate ways. This makes it worth examining whether results for states made of coherent superposition of different particle number also hold for quantum states with fixed particle number.

As mentioned above, physical quantities such as Berry's phase are intricately related to wave functions; it is natural to further inquire whether many-body wave functions constructed from the BdG equations are sufficient for providing information like topological structures of the actual physical states. There are issues beyond fixing particle number. For instance, the BCS ground state wave functions, which can be constructed from the homogeneous BdG equations, do not build in them collective bosonic modes (Anderson-Bogoliubov mode for neutral superconductors and plasmon for charged superconductors [10]) and gauge invariance is violated (for related discussion, see for example [12] - [14]). This is closely related to particle number conservation and plays important roles in quantities such as Berry's phase (cf. Chapter 4).

Aside from concerns with many-body wave functions, we see from the above review that topological properties of Majorana zero modes are deduced without explicitly referring to the underlying many-body wave functions, but rather from properties of solutions to the BdG equations. The artificial particle-hole symmetry of the BdG equations requires the zero energy solutions to be real, which in turns implies the unusual degree of freedom of each localized zero energy solution (or equivalently Majorana zero mode). The resultant non-local entanglement among the spatially separated Majorana zero modes combined with non-interacting quasiparticle picture in the mean-field framework enable us to derive all topological properties of Majorana zero modes in superconductors. It's worth investigating how essential the particle-hole symmetry of the BdG equations and non-interacting single-particle physics are in getting properties of MZM.

As many-body wave functions beyond non-interacting single-particle approximations are extremely difficult to find, if not impossible, it is very helpful to gain some intuitive physical understanding through simple toy models which are constructed as solvable as possible and at the same time contain physics of interest. In order to understand the Berry phase accumulated by moving a localized quasiparticle around a vortex in a superconductor, a basic quantity related to braiding Majorana zero modes, we study a toy model in which relevant degrees of freedom are one dimensional confined in annulus geometry with nontrivial Cooper pair winding number simulating a vortex in actual superconductors. Magnetic flux is threaded through annulus hole to simulate total vortex flux at varying distance to vortex core. We use a local Zeeman field to trap and adiabatically transport a quasiparticle around the annulus and study the Berry phase in such a process. We find that the Berry phase depends on energy spectrum of the system and straightforward application of the BdG equations yields either divergent or mutually inconsistent results. We propose modified many-body wave function ansatz and show that it is necessary to include many-body effect from superconducting condensate and localized quasiparticle interplay.

Inspired by the important role played by superconducting condensate in physics of transporting a quasiparticle around a vortex, we analyze braiding vortices in chiral p-wave superconductors taking into account the condensate for particle number conservation. We find that the condensate effect can be quantitatively accounted for at the mean-field level in the thermodynamic limit for braiding two vortices and the braiding statistics coincide with the standard one, though for more subtle reasons missing in the standard picture. For braiding with at least four vortices that is required for applications to quantum computing, no simple quantitative calculation on the condensate effect is available yet. We then turn to considering the effect of going beyond the mean-field level wave functions. We speculate on the possibility of finite condensate localization/deformation due to the presence of a localized quasiparticle. We further conjecture the possible scenario of local distinguishability of Majorana zero modes induced by particle number conservation through a model involving mesoscopic Josephson junction. Our study shows that more theoretical work is needed in order to establish a more solid basis justifying topological quantum computing with MZM in superconductors.

The thesis is organized as follows. After reviewing in Chapter 2 the mean-field framework underlying the program of topological quantum computing using Majorana zero modes in superconducting systems highlighting key approximations, in Chapter 3 I discuss in some depth aspects of the current framework that may be problematic for deriving the physical properties of interest. I then report our work in attempt to go beyond the BdG framework in Chapter 4 with a toy quasi-1D model to help gain intuitive understanding of the role played by many-body physics in the subject. In Chapter 5, we apply what we have learned from the toy model to study Majorana physics. Finally in Chapter 6, we go over logics of our work and suggest future work towards establishing a more solid theoretical basis beyond the mean-field BdG framework.

Chapter 2

Mean-Field Theory of Majorana Zero Modes in Superconductors and Topological Quantum Computing

In this chapter, we review mean-field theory of Majorana zero modes in superconductors and the application to topological quantum computing. We will not try to exhaust details in this fast growing field, but rather to keep a minimal discussion sufficient for introducing our own work while emphasizing the relevant approximations made in the mean-field framework. We first derive BdG equations and discuss the particle-hole symmetry of BdG solutions in Section 2.1. In Section 2.2, I argue that Majorana zero modes is deduced from the particle-hole symmetry and the non-local entanglement among spatially separated localized Majorana zero modes together with non-interacting quasiparticle approximation give rise to topological protection of qubit formed out of them. Both particle-hole symmetry and non-interacting quasiparticle picture are consequences of mean-field BdG approximation. In Section 2.3, I discuss how Majorana zero modes arise in vortices of chiral p-wave superconductors as consequences of topology of p-wave pairing and vortex winding number and mention how the Cooper pair may make physics more subtle beyond the mean-field picture. In Sections 2.4 and 2.5, I mention other systems people have proposed that make use of superconductivity to create Majorana zero modes. They are all hybrid systems and the bulk superconducting bath has been integrated out in deriving an effective low-energy Hamiltonian which is identical to that of chiral p-wave superconductors. I point out that the treatment also suffers from violation of particle number conservation. So the justification for using these systems for topological quantum computing is subject to similar considerations to that for inherent chiral p-wave superconductors. In the last Section 2.6, I illustrate the derivation of braiding statistics of Majorana zero modes in the mean-field particle number non-conserving framework with the simplest setup of a two-vortex superconductor. We shall later compare the analysis in Section 2.6 to that in Chapter 5 to see how Cooper pair explicitly contributes to the braiding statistics as particle number conservation is enforced.

2.1 BdG Equations

In this section, we review the derivation of BdG equations and their mathematical structures with emphasis on the relevant approximations involved. The starting point is mean-field Hamiltonian after condensing Cooper pairs in superconducting phase. For our purposes, it is sufficient to restrict to spinless fermions and the Hamiltonian is given by

$$\begin{aligned} H &= \int dr \psi^\dagger(r)\hat{H}_0\psi(r) + \frac{1}{2}\int\int drdr' V(r,r')\psi^\dagger(r')\psi^\dagger(r)\psi(r)\psi(r') \\ &= \int dr \psi^\dagger(r)\hat{H}_0\psi(r) + \frac{1}{2}\int\int drdr' \triangle(r,r')\psi^\dagger(r')\psi^\dagger(r) + \frac{1}{2}\int\int drdr' \triangle^*(r,r')\psi(r)\psi(r'), \end{aligned} \tag{2.1}$$

where $\triangle(r,r') \equiv V(r,r')\langle\psi(r)\psi(r')\rangle$ is the superconducting gap that in general depends on location r and r' of two particles, $\psi^\dagger(r)$ and $\psi(r)$ are field operators that create and annihilate a particle at point r respectively. $\hat{H}_0$ is the single-particle energy which is defined relative to chemical potential. I have omitted a constant term on the second line. As we condense Cooper pairs to get superconducting gap on the second line of the above equation to get the mean-field Hamiltonian, particle number conservation (U(1) symmetry) is explicitly broken to Z_2 symmetry (only particle number parity is conserved). We shall see soon that as a result of U(1) symmetry breaking due to mean field approximation, the mean-field Hamiltonian has particle-hole symmetry.

Now since the mean-field Hamiltonian is bilinear in fermion operators, we can diagonalize it through Bogoliubov transformation

$$\psi(r) = \sum_n u_n(r)\alpha_n + v_n^*(r)\alpha_n^\dagger, \tag{2.2}$$

where $\alpha_n^\dagger$ are Bogoliubov-deGennes quasiparticle creation operators that diagonalize the mean-field

Hamiltonian

$$H_{MF} = \sum_n E_n \alpha_n^\dagger \alpha_n. \tag{2.3}$$

Making use of the commutation relation of $\alpha_n^\dagger$ and α_n with H_{MF}

$$\begin{aligned} [H, \alpha_n] &= -E_n \alpha_n \\ [H, \alpha_n^\dagger] &= E_n \alpha_n^\dagger \end{aligned} \tag{2.4}$$

and commutation relation of field operators $\{\psi(r), \psi(r')\} = \{\psi^\dagger(r), \psi^\dagger(r')\} = 0$ and $\{\psi(r), \psi^\dagger(r')\} = \delta(r - r')$, we obtain two equations for $[H, \psi(r)]$

$$[H, \psi(r)] = \sum_n -u_n(r) E_n \alpha_n + v_n^*(r) E_n \alpha_n^\dagger \tag{2.5}$$

and

$$\begin{aligned} [H, \psi(r)] &= -\hat{H}_0 \psi(r) + \frac{1}{2} \int dr' (\triangle(r, r') - \triangle(r', r)) \psi^\dagger(r') \\ &= -\hat{H}_0 (\sum_n (u_n(r) \alpha_n + v_n^*(r) \alpha_n^\dagger) + \int dr' \triangle (r, r') \sum_n (u_n^*(r') \alpha_n^\dagger + v_n(r') \alpha_n). \end{aligned} \tag{2.6}$$

Comparing RHS of equation (2.5) with equation (2.6), we obtain the equations for $u_n(r)$ and $v_n(r)$

$$\begin{aligned} \hat{H}_0 u_n(r) - \int dr' \triangle (r, r') v_n(r') &= E_n u_n(r) \\ \int dr' \triangle^* (r, r') u_n(r') - \hat{H}_0^* v_n(r) &= E_n v_n(r). \end{aligned} \tag{2.7}$$

These are the BdG equations for general spinless superconductors. Now let's specify to p+ip pairing and simplify equation (2.7). To simplify pairing terms, it is customary to assume that center of mass and relative degrees of freedom are separable and $\triangle(r, r')$ is simplified to

$$\triangle(r, r') = - \triangle (R) i(\bigtriangledown_x + i\bigtriangledown_y)\delta(\bar{r}), \tag{2.8}$$

where R and $\bar{r}$ are center of mass and relative coordinates respectively. Substituting the expression for $\triangle(r, r')$ into the general form of the BdG equations (2.7), we obtain the BdG equations for p+ip superconductors:

$$\begin{aligned} \hat{H}_0 u(r) - i \triangle(r)(\bigtriangledown_x + i\bigtriangledown_y)v(r) &= Eu(r) \\ -i \triangle^*(r)(\bigtriangledown_x - i\bigtriangledown_y)u(r) - \hat{H}_0^* v(r) &= Ev(r). \end{aligned} \tag{2.9}$$

Note that equation (2.9) has the symmetry

$$\begin{aligned} \sigma_1^\dagger H_{\mathrm{BdG}} \sigma_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} H_0 & \triangle(k_x + ik_y) \\ \triangle^*(k_x - ik_y) & -H_0^* \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \triangle(k_x + ik_y) & H_0 \\ -H_0^* & \triangle^*(k_x - ik_y) \end{pmatrix} \\ &= \begin{pmatrix} -H_0^* & \triangle^*(k_x - ik_y) \\ \triangle(k_x + ik_y) & H_0 \end{pmatrix} \\ &= -H_{BdG}^*, \end{aligned} \tag{2.10}$$

where $k_x = -i\partial_x$ and $k_y = -i\partial_y$.

So if $(u(r), v(r))^T$ is a solution to (2.9) with eigenvalue E, then $(v^*(r), u^*(r))^T$ is also a solution with eigenvalue $-E$. This particle-hole symmetry is a result of mean-field approximation which puts creating and annihilating a particle (or equivalently creating a hole) on the same footing as the difference between particle and hole respects Z_2 symmetry of mean-field Hamiltonian and is absorbed into Cooper pair condensate which is taken as classical field. Note that the particle-hole symmetry of the BdG equations is independent of the assumption (2.8), although for simplicity, I have used it and the resulting BdG equations (2.9) for the proof. One can start from equation (2.7) and get the same result. This symmetry can also be seen from the expression of $\alpha^\dagger$, which can be found from equation (2.2)

$$\alpha^\dagger = \int dr u_n(r)\psi^\dagger(r) + v_n(r)\psi(r) \tag{2.11}$$

as its Hermitian conjugate α corresponds to eigenvalue with opposite sign

$$\alpha = \int dr v_n^*(r)\psi^\dagger(r) + u_n^*(r)\psi(r). \tag{2.12}$$

We'll see in the next section that this particle-hole symmetry is of crucial importance in deducing Majorana zero modes.

2.2 Physical Properties of Majorana Zero Modes

I now discuss physical properties of Majorana zero modes in superconductors relevant to their applications to topological quantum computing and show how these properties are derived from the mean-field approximation and the BdG equations. Here I focus on indistinguishability and non-local quantum entanglement of Majorana zero modes. I'll leave non-Abelian braiding to the last section for a separate discussion.

It's straightforward to show that the existence of the Majorana zero modes can be deduced from the particle-hole symmetry of the BdG solutions provided there exist zero energy solutions. If $(u(r), v(r))^T$ is solution to (2.9) with eigenvalue 0, then $(v^*(r), u^*(r))^T$ is also solution with eigenvalue 0. For two BdG solutions (in p+ip superconducting pairing) that are connected by particle-hole symmetry, they correspond to creation and annihilation of the same Bogoliubov quasiparticle with positive energy (see equation 2.11 and 2.12). In the special case where the corresponding eigenvalue is zero, we can no longer distinguish creation from annihilation (or put it another way, creating a particle and creating a hole, i.e., annihilating a particle, is the same thing, at least locally), so the corresponding pair of solutions must be the same solution. So we have $v^*(r) = u(r)$ and $u^*(r) = v(r)$. From (2.11) and (2.12), we get the defining property of Majorana fermions

$$\gamma^\dagger = \gamma, \tag{2.13}$$

where I have relabeled α with γ, which is conventionally used to denote Majorana fermions.

We see above that the zero energy solutions to the BdG equations (2.9) imply the existence of Majorana zero modes as a result of the particle-hole symmetry. Now let's show that if these Majorana zero modes are localized in space, the degenerate ground states related by them are locally indistinguishable. For illustration, I consider the simplest case with doubly degenerate ground states related by a single zero energy Dirac fermion. (Dirac fermion in the sense of satisfying Fermi statistics. It is equivalent to another name: complex fermion if we call a Majorana fermion real fermion. In the following, the word "Dirac fermion" or "Dirac mode" all has the same meaning.) Since Majorana fermions don't themselves satisfy Fermi statistics, we need at least a pair of them to form a Dirac fermion. So a zero energy Dirac mode can be formed by

$$\alpha^\dagger = \frac{1}{2}(\gamma_1 + i\gamma_2), \tag{2.14}$$

where γ_1 and γ_2 are two Majorana zero modes each of which is localized around position r_1 and r_2 that are separated in space from each other. The factor 1/2 is for normalization condition of the Dirac fermion and the relative phase factor between two Majorana fermions can be either i or $-i$ for the Dirac fermion to satisfy Fermi statistics. We choose i here for Dirac fermion creation operator acting on one ground state. If we instead choose $-i$, then the corresponding Dirac fermion creation operators will be acting on the other ground state. The conclusion is of course independent of the choice. Let's denote the two ground states $|0\rangle$ and $|1\rangle$ that are related by

$$|1\rangle = \alpha^\dagger|0\rangle. \tag{2.15}$$

Consider now an arbitrary local Hermitian operator $\hat{\Omega}(r_0) = \hat{\Omega}^\dagger(r_0)$ (since only Hermitian operators correspond to physical observables) localized around r_0 and evaluate its matrix elements within the doubly degenerate ground state subspace. The diagonal elements are related by the following equation

$$\langle 1|\hat{\Omega}(r_0)|1\rangle = \langle 0|\alpha\hat{\Omega}(r_0)\alpha^\dagger|0\rangle. \tag{2.16}$$

If r_0 is far from both r_1 and r_2 where Majorana zero modes are localized, then we can evaluate the RHS of the above equation by commuting $\hat{\Omega}(r_0)$ with $\alpha^\dagger$ which vanishes and we get

$$\langle 0|\alpha\hat{\Omega}(r_0)\alpha^\dagger|0\rangle = \langle 0|\hat{\Omega}(r_0)|0\rangle + \langle 0|\alpha[\hat{\Omega}(r_0), \alpha^\dagger]|0\rangle = \langle 0|\hat{\Omega}(r_0)|0\rangle. \tag{2.17}$$

So the diagonal elements are the same $\langle 0|\hat{\Omega}(r_0)|0\rangle = \langle 1|\hat{\Omega}(r_0)|1\rangle$ for r_0 far from both Majorana zero modes.

If r_0 is close to one of the Majorana zero modes, say r_2, we need to make use of the fact that $|0\rangle$ is annihilated by α, i.e., $\alpha|0\rangle = 1/2(\gamma_1 - i\gamma_2)|0\rangle = 0$, to relate the two degenerate ground states by the other Majorana mode and rewrite (2.15) as

$$|1\rangle = \gamma_1|0\rangle. \tag{2.18}$$

Substituting (2.18) into (2.16) and commuting $\hat{\Omega}(r_0)$ with γ_1 which vanishes, we arrive at the same result $\langle 0|\hat{\Omega}(r_0)|0\rangle = \langle 1|\hat{\Omega}(r_0)|1\rangle$.

For the off-diagonal element, it vanishes trivially for the degenerate ground states considered here as they have different particle number parity. For physically more interesting case of degenerate ground states with the same particle number parity, the system much contain at least two zero energy Dirac modes. The evaluation can proceed similarly to what we did above for the diagonal elements. As the two zero energy Dirac modes are split among four Majorana zero modes that are spatially separate from each other, we can focus on one of the Dirac zero modes near which the local hermitian operator probes. For notation simplicity, we adopt the same notation as above for the degenerate ground states and we call the relevant Dirac zero mode creation operator $\alpha^\dagger$ omitting writing down the other Dirac zero mode explicitly. The off-diagonal element is similarly evaluated as

$$\begin{aligned}\langle 0|\hat{\Omega}(r_0)|1\rangle &= \langle 0|\hat{\Omega}(r_0)\alpha^\dagger|0\rangle \\ &= \langle 0|\alpha^\dagger\hat{\Omega}(r_0)|0\rangle + \langle 0|[\hat{\Omega}(r_0), \alpha^\dagger]|0\rangle \\ &= 0. \end{aligned} \tag{2.19}$$

Since the off-diagonal elements vanish and the diagonal elements are identical, no local Hermitian operator can distinguish the two degenerate ground states. In the above derivation leading to the indistinguishability of degenerate ground states, we rely on the assumption that ground states are eigenstates of occupation number of zero energy Dirac fermions which are split non-locally at physically separate regions where localized Majorana zero modes reside. This is true for an effective non-interacting (quasi-)particle picture obtained from the mean-field approximation and the BdG equations. In Chapter 5, we shall examine whether when many-body effect is taken into account, the property of indistinguishability still survives. There's no a priori reason to believe that it is the case.

Since degenerate ground states are locally indistinguishable, we say they are topologically protected from the environment as physical perturbations from the environment are all local in space (of course, we are talking about low energy physics and we assume there is energy gap that separates degenerate ground states from excited states). In the last section, we shall see that the only way to introduce non-trivial transform within the ground state subspace is through braiding these Majorana zero modes with resulting states depending only on the topology of braiding trajectories, hence the name topological quantum computing when we use these ground states as effective qubits and braiding as gate operations.

Before leaving the section, I want to briefly comment on the non-local quantum entanglement of Majorana zero modes. In the above discussion of indistinguishability, we see that $\gamma_1|0\rangle = i\gamma_2|0\rangle$ (see discussion right above equation (2.18)) which says that operators that are localized at separate regions yield the same wave function when acting on the ground state, indicating non-local quantum entanglement between Majorana zero modes and in the ground state wave functions. It's interesting to observe the analogy to maximum entangled states which play a important role in quantum information. For instance a Bell state is maximal entangled at two separate places and locally no useful quantum information is available.

2.3 Majorana Zero Modes in Vortices of Chiral P-wave Superconductors

Now I discuss Majorana zero modes in vortices of p+ip superconductors. There is not much sense to give here detailed derivation of Majorana solutions to the BdG equations localized in vortices of p+ip superconductors as it has been well established and thoroughly discussed in literature (e.g. [15] - [17]). Instead, I'll focus on conceptual aspect of the existence of Majorana zero modes as consequence of topological features of chiral superconductors in the presence of vortices, which is most relevant to the topics discussed in the thesis.

There has been proof (e.g. [18]) on the existence of Majorana zero modes in vortices based on the usual assumption that the center of mass and relative coordinates of gap function can be separated, i.e., the BdG equations take the form (2.9). The system is then reduced to an effective one dimensional system with a mass domain wall at the vortex and standard argument due to Jackiw and Rebbi [19] can be applied to show the existence of zero energy local mode. Here I take a slightly more general approach to emphasize the topological feature. I shall not rely on the separability assumption of the gap function at the price of providing more heuristic and weaker argument about the existence of Majorana zero modes, namely I can only provide necessary conditions for their existence. Nevertheless, the discussion highlights the key component for the existence of Majorana zero modes and furthermore raises interesting issues when superconducting condensate is explicitly taken into account (the latter will be delayed to the next chapter when we discuss particle number conservation in more details).

Consider first an isolated vortex located at the origin. The solutions to the BdG equations (2.7) can be chosen to correspond to eigenstates of angular momentum in the sense that both $u(r)$ and $v(r)$ are eigenstates of angular momentum with eigenvalues differing by the angular momentum of the Cooper pair or equivalently the gap function. It's easy to check that such $u(r)$ and $v(r)$ is consistent with the BdG solutions. Explicit calculations indeed confirm that the angular momentum condition is satisfied by the BdG solutions.

Now what constraint does existence of Majorana zero mode put on the angular momentum? Since $u(r) = v^*(r)$ for a Majorana solution, the angular momentum of $u(r)$ must be opposite to that of $v(r)$. To satisfy BdG equations as given by 2.9, the difference of angular momentum for $u(r)$ and $v(r)$ must equal to angular momentum associated with local superconducting order parameter. Therefore the magnitude of angular momentum of $u(r)$ and $v(r)$ must equal one half of that of the order parameter. Namely, since $l_u - l_v = l_c$, and $l_u = -l_v$, so $|l_u| = |l_v| = l_c/2$. l_u, l_v and l_c denote angular momentum quantum number of $u(r)$, $v(r)$ and local order parameter, respectively. Since both $u(r)$ and $v(r)$ need to satisfy single-valued condition, their angular momentum quantum number can only be integer. Hence we arrive at the necessary condition for the angular momentum of the local order parameter. It can only take even integers. For p+ip superconductors, a vortex with single flux quantum $h/2|e|$ (and more generally odd flux quanta) satisfies this condition (the intrinsic angular momentum due to p+ip pairing is one and the angular momentum due to vorticity is one for $h/2|e|$ flux, the sum of the two contribution is even). The exponential localization of Majorana zero modes then follows from the fact that the bulk is gapped.

Finally, I would like to briefly mention the splitting of degenerate ground states in systems with finite size and the fate of Majorana zero modes. Our discussion on Majorana zero modes above takes into account only one vortex without the effect of the other which is accurate to within exponential small error when the spatial separation of the two vortices is much larger than the size of each localized Majorana zero mode. As we take into account the overlap of two localized Majorana zero modes at two vortices, the energy level of the Dirac fermion excitation formed out of the two localized Majorana modes becomes finite though exponentially close to zero. Notice that there is still a single energy level out of the two localized Majorana modes and it is shifted from zero to small positive value when system finite size effect is taken into account. The crucial physical property that make Majorana zero modes topologically nontrivial is not their exact zero energy level which is never realized in any realistic system but their sharing physical degrees of freedom among spatially separated modes.

2.4 Kitaev Wire - A Toy Model

Perhaps the simplest model system giving rise to Majorana zero modes in superconductors is one dimensional Kitaev wire [8]. This models is exactly solvable with all essential physics of Majorana zero modes included. Consider a one dimensional normal wire with non-interacting spinless fermions deposited on the surface of a bulk superconductor with p-wave pairing as shown in figure 2.1. Due to proximity effect, off-diagonal long range order is induced in the 1D wire with order parameter of the same form as that of the bulk superconductor. If we approximate the effective Hamiltonian of the 1D wire to be the BCS mean-field Hamiltonian that breaks particle number conservation and neglect the interaction between the wire and the bulk except that the bulk provides stationary off-diagonal long range order to the wire, we will find that the wire possesses topologically nontrivial phase in which there are localized Majorana zero modes localized at each end of the wire. For example, consider the following Hamiltonian

$$H_{\mathrm{kw}} = \sum_{i=1}^{N-1} -a_i^\dagger a_{i+1} + a_i^\dagger a_{i+1}^\dagger + h.c., \tag{2.20}$$

where lattice sites runs from 1 to N, $a_i^\dagger$ is create a fermionic particle at site i. The chemical potential is tuned to zero so the wire is half filled in the normal state. The superconducting gap is tuned to have the same magnitude as hopping strength. In this special case, we get Majorana zero modes localized at each end of the wire, i.e., at site 1 and N, respectively. This can be mostly easily seen by rewriting fermion creation and annihilation operators in terms of Majorana operators, i.e., we express $a_i^\dagger$ and a_i as

$$\begin{aligned} a_i^\dagger &= \frac{1}{2}(\gamma_{iA} + i\gamma_{iB}) \\ a_i &= \frac{1}{2}(\gamma_{iA} - i\gamma_{iB}), \end{aligned} \tag{2.21}$$

where γ_{iA} and γ_{iB} are Majorana operators satisfying $\gamma_{iA}^2 = \gamma_{iB}^2 = 1$, $\{\gamma_{iA}, \gamma_{jB}\} = 0$. Substituting 2.21 into 2.20, we can rewrite the Kitaev Hamiltonian in basis of Majorana operators

$$H_{\mathrm{kw}} = \sum_{i=1}^{N-1} i\gamma_{iB}\gamma_{i+1,A}. \tag{2.22}$$

In this form, we can readily see that there are two Majorana operators absent in the Hamiltonian, γ_{1A} and $\gamma_{N,B}$. They commute with the Kitaev Hamiltonian and hence are zero modes. More generally, the existence of Majorana zero modes at wire ends is guaranteed as the transition point between topologically nontrivial bulk phase in the wire and trivial phase outside the wire, i.e., vacuum and their localization near the ends is due to the wire bulk gap.

It should be always kept in mind that they are not independent physical degrees of freedom and the physical zero mode is formed by combining them as real and imaginary part. In other words, each zero energy Majorana fermion should be regarded as linear combination of a physical zero energy fermion creation operator and an annihilator (which is the hermitian conjugate of the zero energy fermion annihilation operator) annihilating the ground state to which it is acting on.

The existence of Majorana zero modes relies on the factorization between the wire and the bulk superconductor in the sense that we can neglect the effect from the coupling of the wire to the bulk superconductor. The justification of this assumption is lacking. In particular, from the perspective of using these modes for quantum information processing and computing, we should really consider the wire and the bulk together as our system that explicitly conserves total particle number as the relevant physical states that comprise qubit have fixed fermion numbers.

2.5 Other Hybrid Systems Utilizing Superconductivity

Various hybrid systems harboring Majorana zero modes have been proposed. They all share the same effective low energy Hamiltonian, namely, the BCS mean-field particle number non-conserving Hamiltonian with effective p+ip pairing. In this sense, all systems are physically equivalent to the p+ip superconductors with difference only in physical conditions in realizing the effective Hamiltonian. Also they all rely on the proximity effect to a bulk superconductor whose dynamics is neglected and whose sole role is to supply a static superconducting order parameter to the system of interest. Therefore they all need proper justification of particle number non-conserving approximation. For example, as we consider the state of the whole "universe" (system + bath) which has fixed total particle number, the local modification of bath due to the system also needs to be taken into account which is always neglected in the mean-field framework.

2.6 Braiding Majorana Zero Modes

Now let's describe properties of Majorna zero modes under braiding in the mean-field particle number non-conserving framework. For our purposes, we will only consider the simplest case of interchanging two localized Majorana zero modes in a superconductor in the presence of two vortices. We shall compare the overall phase change (which is also called holonomy) of the doubly degenerate ground states after the interchange. In the more relevant case with at least four localized Majorana zero modes, we can always choose to work in a diagonal ground state basis where interchanging the two MZM we consider doesn't mix basis states and compare the relative overall phases for the two basis states after the interchange. (We need at least four vortices because degenerate ground states in a system with two vortices and so two MZM have different particle number parity and they can not transform into each other under interchanging two MZM. To realizing degenerate ground states with same particle number parity, we need at least four MZM and two Dirac Bogoliubov zero modes. Four MZM permit ground states to mix into each other under braiding MZM and is useful for qubit operation.) If the relative phase is non-zero (modulo 2π), then we can conclude that the interchange can induce a nontrivial unitary transformation in the ground state space for the following reason. Suppose we choose our initial states to to be different from diagonal basis states and consider their evolutions under the same braiding process for the diagonal basis ground states. Each one of them will evolve into linear combinations of their initial states since each of them is linear combinations of the diagonal basis ground states and different phases picked up by the two basis ground states are going to change the relative coefficients in the linear combinations, driving each of them out of themselves. We will see below that the BdG theory predicts non-trivial relative phase and thus we call the non-trivial unitary evolution of ground states by saying that Majorana zero modes obey non-Abelian statistics. All essential physics is already captured in the simplest case considered here without loss of generality.

Consider interchanging vortex 2 with vortex 1, as shown in figure 2.2. Each vortex harbors a Majorana zero mode. Define the two degenerate ground states, one with even particle number state $|0(\theta_0)\rangle$ and the other with odd particle number state $|1(\theta_0)\rangle$ created from $|0(\theta_0)\rangle$ by the adding a zero energy BdG quasiparticle

$$\alpha^\dagger = \frac{1}{2}(\gamma_1 + i\gamma_2) \tag{2.23}$$

with γ_1 and γ_2 Majorana zero mode operators sitting in vortex 1 and 2 respectively, given by

$$\gamma_i(\theta_0) = \int d^2r u_i(r,\theta_0)\psi^\dagger(r) + v_i(r,\theta_0)\psi(r), \tag{2.24}$$

where $i = 1, 2$ and $u_i(r,\theta_0) = v_i^*(r,\theta_0)$ are functions localized in vortex i. The normalization condition for $u_i(r,\theta_0)$ is $\int d^2r\, |u_i(r,\theta_0)|^2 = 1$. θ_0 is a parameter characterizing the position of the vortex pair (see figure (2.2)) with initial value 0 and final value π after interchange.

Since after the interchange, the system Hamiltonian goes back to the initial one before the interchange, the instantaneous ground states $|0(\theta_0)\rangle$ and $|1(\theta_0)\rangle$ must go back to their initial states up to some phases which is called monodromy phase. In the adiabatic limit, each ground state will evolve back to itself at the end of the interchange up to overall phases. They wouldn't evolve to linear superposition of the two basis ground states as the basis states have different particle number parity. In the more relevant case of four Majorana zero modes, the relevant basis ground states have same particle number parity. There, we need to calculate the matrix of Berry connection. If we choose our initial states (which coincide with our basis states) properly, we can always make the matrix diagonal so that we only need to consider Berry phases associated with our states. There are two contributions to the overall relative phase accumulated by the two ground states. The first is from the monodromy phase, i.e.

$$\begin{aligned} |0(\pi)\rangle &= e^{i\alpha_0}|0(0)\rangle \\ |1(\pi)\rangle &= e^{i\alpha_1}|1(0)\rangle. \end{aligned} \tag{2.25}$$

The second is from the Berry phase,

$$\begin{aligned}
\phi_0 &= -\mathrm{Im}\{\int_0^\pi d\theta_0 \langle 0(\theta_0)|\partial_{\theta_0}|0(\theta_0)\rangle\} \\
\phi_1 &= -\mathrm{Im}\{\int_0^\pi d\theta_0 \langle 1(\theta_0)|\partial_{\theta_0}|1(\theta_0)\rangle\}.
\end{aligned} \tag{2.26}$$

The total relative phase is equal to

$$\chi = \delta\alpha + \delta\phi, \tag{2.27}$$

where $\delta\alpha \equiv \alpha_1 - \alpha_0$ and $\delta\phi = \phi_1 - \phi_0$.

The Majorana wave functions $u_i(r, \theta_0)$ can be written as [17]

$$\begin{aligned}
u_1(r, \theta_0) &= \exp\{\frac{(\pi + \theta_0)i}{2}\}u(|\vec{r} - \vec{R}_1|)e^{i\theta(\vec{r}-\vec{R}_1)} \\
u_2(r, \theta_0) &= \exp\{\frac{\theta_0 i}{2}\}u(|\vec{r} - \vec{R}_2|)e^{i\theta(\vec{r}-\vec{R}_2)},
\end{aligned} \tag{2.28}$$

where $\theta(\vec{r} - \vec{R}_i)$ is polar angle of vector $\vec{r} - \vec{R}_i$, $\vec{R}_i$ is the location of vortex i (i=1,2). The overall phases dependent on θ_0 for u_1 and u_2 come from overall phases of gap function near each vortex due to the superconducting phase induced by the other vortex. The superconducting phase increases by 2π going around each vortex counter-clockwisely. The overall superconducting phase at vortex 1 is $\pi + \theta_0$ and θ_0 at vortex 2 (see figure 2.2 for vortex configuration, we define zero phase in the positive x direction). So the overall phases for u_1 and u_2 are $(\pi + \theta_0)/2$ and $\theta_0/2$, respectively (cf. BdG equations (2.9)). The azimuthal dependence of u_1 and u_2 is given by phases of azimuthal angles $\theta(\vec{r} - \vec{R}_1)$ and $\theta(\vec{r} - \vec{R}_2)$ since u_1 and u_2 are eigenstates of angular momentum (with eigenvalue one) with respect to their associated vortices.

After the interchange, θ_0 goes from 0 to π, we have by (2.28)

$$\begin{aligned} u_1(r,\pi) &= -u_2(r,0) \\ u_2(r,\pi) &= u_1(r,0) \\ \alpha^\dagger(\pi) &= i\alpha^\dagger(0). \end{aligned} \tag{2.29}$$

Combining (2.29) with the definition of the instantaneous ground states, we get the monodromy phase

$$\delta\alpha = \pi/2. \tag{2.30}$$

Now let's calculate the Berry phase. It is

$$\begin{aligned} \delta\phi &= -\mathrm{Im}\{\int_0^\pi d\theta_0 \langle 1(\theta_0)|\partial_{\theta_0}|1(\theta_0)\rangle - \int_0^\pi d\theta_0 \langle 0(\theta_0)|\partial_{\theta_0}|0(\theta_0)\rangle\} \\ &= -\mathrm{Im}\{\int_0^\pi d\theta_0 \langle 0(\theta_0)|\alpha(\theta_0)[\partial_{\theta_0}, \alpha^\dagger(\theta_0)]|0(\theta_0)\rangle\} \\ &= -\mathrm{Im}\{\int_0^\pi d\theta_0 \langle 0(\theta_0)|\alpha(\theta_0)(\partial_{\theta_0}\alpha^\dagger(\theta_0))|0(\theta_0)\rangle\} \\ &= -\mathrm{Im}\{\int_0^\pi d\theta_0 \langle 0(\theta_0)|\{\alpha(\theta_0), (\partial_{\theta_0}\alpha^\dagger(\theta_0))\}|0(\theta_0)\rangle\}. \end{aligned} \tag{2.31}$$

It's straightforward to show that the contribution from derivatives of $u_i(r,\theta_0)$ and $v_i(r,\theta_0)$ vanishes and so $\delta\phi = 0$. This is due to two characteristics of localized Majorana zero modes: reality condition of γ_i so that $u_i = v_i^*$; u_1 and u_2 are localized at separate regions so their overlap is exponentially small. As we'll see in Chapter 5, once the Cooper pair operator is added to BdG quasiparticle operator, γ_i are no longer real and they are affected by the Cooper pair during the braiding. Furthermore, there can be contribution to the Berry phase from the Cooper pair.

Combining 2.30 with vanishing relative Berry phase, the total relative phase is

$$\chi = \pi/2 + 0 = \pi/2. \tag{2.32}$$

This is the standard result first derived by Ivanov [7]. We see that after interchanging vortex 1 with

2, the evolution of the two ground states picks up different overall phases and the phase difference is $\pi/2$. The contribution comes only from the monodromy phase.

2.7 Figures

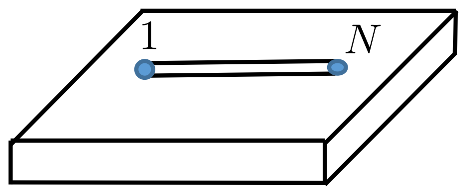

Figure 2.1: Kitaev wire formed by depositing a normal wire on bulk superconductor with p-wave pairing. Sites 1 and N are located at two ends.

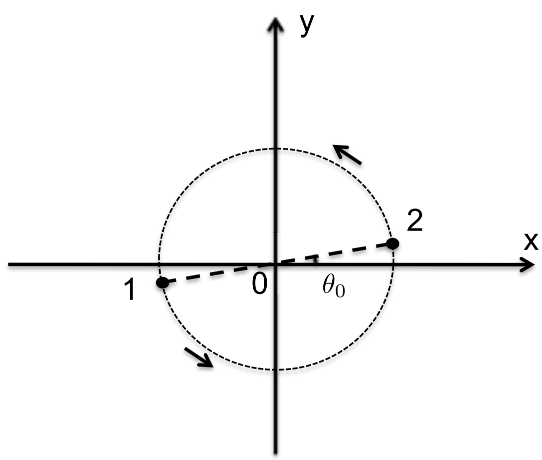

Figure 2.2: Configuration of braiding two vortices. The dashed circle centered around 0 with arrows indicates the trajectories of vortices 1 and 2 during the counter-clockwise exchange. θ_0 parameterizes the position of the two vortices.

Chapter 3

Conceptual Issues with Mean-Field Approximations

In the previous chapter, we've seen how Majorana zero modes and its topological properties are derived from the mean-field approximations. In this chapter, we explore conceptual issues on using mean-field approximations and BdG equations to deduce properties of Majorana zero modes for quantum information and quantum computing purposes. We will argue that the main issue with the mean-field treatment is the violation of particle number conservation which is conceptually inconsistent with fundamental requirement on quantum states for quantum information and quantum computing (Section 3.1.1) and also results in unphysical consequences such as violation of gauge invariance and f-sum rule (Section 3.1.2) (as illustrated in particular by an example of incorrect prediction on experimental signature in NMR of ^{3}Helium-B phase surface in Section 3.1.2.1 based on naive mean-field approximations) and Galilean invariance (Section 3.1.3). In Section 3.2, I'll discuss the effect of particle-hole symmetry as a consequence of mean-field BdG approximation on Majorana zero modes. Finally in Section 3.3, I mention a subtle point between BdG equations and many-body states.

3.1 Particle Number Conservation

3.1.1 Pure versus Mixed States

We know that physical states that form qubits need to be pure quantum states. On the other hand, many-body ground states corresponding to the BdG equations are coherent superpositions of quantum states with different fermion numbers. These ground states do not correspond to pure quantum states in physical systems which always have fixed electron numbers. The exotic coherent superposition of different fermion numbers is a mere artifact of BCS mean-field trick in which particle number conservation is relaxed for ease of mathematical treatment, but not for physical reasons. This is rather obvious for an isolated superconductor (in the sense that no conducting lead is attached to it) where total electron number is fixed. For hybrid systems mentioned in Section 2.4 and 2.5 where the interesting physics appears to occur only in part of the whole system, for example, for a Kitaev wire, the rest of the system, i.e., bulk superconductor, seems unimportant and can be integrated or traced out. However, a basic argument shows that it is not true. Consider the density matrix of a hybrid system in a pure quantum state given by

$$\hat{\rho}_t = |\psi\rangle\langle\psi|. \tag{3.1}$$

The state $|\psi\rangle$ can be written as superposition of tensor product of state of the system of interest (for instance, the Kitaev wire) called 's' and state of the rest of the hybrid system, called environment 'e', i.e.,

$$|\psi\rangle = \sum_{ij} \alpha_{ij} |s_i\rangle \otimes |e_j\rangle. \tag{3.2}$$

Tracing over the environment, we get the reduced density matrix for s

$$\hat{\rho}_s = \sum_{ii'j} \alpha^*_{ij} \alpha_{i'j} |s_i\rangle\langle s_{i'}|. \tag{3.3}$$

If we choose the basis state $|e_i\rangle$ to be eigenstate of particle number, i.e., each state has definite particle number, then the basis state of the system $|s_i\rangle$ has to have definite particle number as well since the total particle number is constant. As indicated by each coefficient (i.e. $\alpha^*_{ij}\alpha_{i'j}$) in the reduced density matrix $\hat{\rho}_s$ corresponding to $|s_i\rangle\langle s_{i'}|$ as the sum over the same index j for the environment basis state, $|s_i\rangle$ and $\langle s_{i'}|$ must have the same particle number otherwise the two states correspond to different total particle number of the universe. So the reduced density matrix is diagonal in the particle number basis and can not contain coherent superposition of states with different particle numbers. This means if we trace out the environment, we are not going to get pure quantum states as superposition of states with different particle numbers. So in any case, we really need to consider states with fixed particle number.

The physical effect on Majorana zero modes brought by fixing total particle number can be illustrated in a simple example of a p+ip superconducting state with two vortices having the same winding number. For this purpose, we extend our discussion on Majorana zero modes in vortices from Section 2.3. Recall that we explain from topology in that section the necessary condition for local superconducting order parameter topology (i.e., local winding number or equivalently angular momentum) to enable existence of Majorana zero modes. We have considered only one local Majorana zero mode. Now we complete the discussion by considering one Dirac zero mode which requires account of another Majorana zero mode, either sitting at another vortex or bound to system boundary (if there is only one vortex in the system). Let's consider the former case where the presence of another vortex changes topology of system state. The analysis of Majorana zero mode in one vortex in Section 2.3 is unaffected by including multiple vortices since each mode is exponentially localized and locally the gap function looks the same except for an overall phase due to the other vortex. So the second vortex appears to be innocuous to our argument. However, there is an interesting issue if we recover particle number conservation. The full Hamiltonian (without mean-field approximation, cf. the first line of equation (2.1)) approximately commutes with angular momentum if the two vortices are close to the origin and the system size approaches thermodynamic limit. Since both ground states are eigenstates of total particle number with different eigenvalues differed by one and total particle number commutes with angular momentum, they must be eigenstates of angular momentum too. Because if they were not, the angular momentum operator acting on them will mix them and the resulting states would no longer be eigenstates of total particle number. Note that angular momentum operator can't mix energy eigenstates with same particle number since these eigenstates much have different energy eigenvalues (but we know angular momentum acting on an energy eigenstate must yield an energy eigenstate with same energy eigenvalue due to commutativity of Hamiltonian and angular momentum). Now let's assume the two degenerate ground states are still approximately related to each other by a zero energy (modulo chemical potential) Bogoliubov quasiparticle whose form is given by solutions to the BdG equations. Since both ground states have fixed particle number, we need to explicitly add a Cooper pair associated to the hole component of the Bogoliubov quasiparticle to satisfy particle number conservation. Since the angular momentum of the Cooper pair is three, the angular momentum associated to the hole component can not be the same as that of the particle component since the difference of angular momentum of hole and particle component can only be even (for this point, refer to discussion in Section 2.3) for Majoranas. This implies that the particle number conserved BdG quasiparticle is not eigenstate of angular momentum and therefore the two degenerate ground states can not both be eigenstate of angular momentum and we reach a paradox. Of course, as the full Hamiltonian doesn't conserve angular momentum exactly, the above argument doesn't reach a rigorous paradox. Nevertheless, we notice that the average angular momentum of a Majorana zero mode is two in particle number non-conserving approximation, whereas it is $2+\frac{3}{2}=7/2$ as we take into account the Cooper pair associated with quasiparticle hole in particle number conserving treatment. The angular momentum of Cooper pair has interesting contribution to the Berry phase as we shall see in Section 5.2.1.2.

We note here that although there has been interesting work on Majorana physics in particle number conserving systems (e.g. [20]- [26]), none of them strictly addresses superconductors with conserved particle number.

3.1.1.1 Braiding MZM using Kitaev Wire Networks with Fixed Particle Number

The particle number conservation may be enforced at different levels. At the most naive level, we may simply project a BdG many-body ground state to constant particle number sectors and ask whether the properties derived for the BdG ground state survive in each fixed particle number sector. Even this simple-looking problem turns out to be non-trivial as we will see in Section 5.2. The fundamental difficulty comes from lack of knowledge of many-body wave functions. It is thus natural to seek model systems where simple analytic form of many-body wave functions can be found. Kitaev wire is the ideal model system where we know everything about many-body eigenstates. So we can explicitly calculate properties like Berry phase for each fixed particle number sector. Of course, in the case of Kitaev wires, each fixed particle number sector should correspond to projecting many-body ground state wave function of the whole system (wire + superconducting bath). Nevertheless, we'll pretend that the Kitaev wire is inherently superconducting, for example, we may regard the wire as a chain in a quasi-1D superconductor. In order to calculate braiding properties, we need to consider some network of Kitaev wires and interchange two end Majorana zero modes [27]. We have performed such calculations for two cases. In one case, we realized double interchange of two MZM during which the two degenerate ground states are kept real. So there's no Berry phase for either of them. Particle number conservation doesn't pose any new issue. In the other case, we performed single interchange of two MZM. For ease of calculation, we switch to a basis where two degenerate ground states are kept real during the interchange but they evolve into each other at the end of interchange. We then calculate off-diagonal Berry phase for each particle number sector. Interestingly, not all sectors have the same Berry phase. The two states in sector which corresponds to average particle number have the same Berry phase, whereas states in other sectors have different Berry phases. This poses a problem of particle-number non-conserving scheme. Since in the particle number non-conserving scheme, the result of braiding is completely insensitive to average particle number. We can assign even non-integer average particle number without affecting the braiding result. As we project the result onto each particle number sector, we may get braiding result different from the average! For more details of calculations, refer to Appendix A.

3.1.2 Gauge Invariance and f-sum Rule

The BCS mean-field theory and the corresponding reduced BCS Hamiltonian violates gauge invariance and it is a subject under intensive debate in early days of BCS theory. It is realized that collective modes of condensate need to be included to restore gauge invariance and various sum rules such as f-sum rule. In the case of translational invariant BCS Hamiltonian, pair interaction with non-zero center of mass momenta needs to be included as shown by Anderson to enforce gauge invariance and we get low energy collective excitations such as Anderson-Bogoliubov mode for neutral superconductors. It is interesting to ask how this modification beyond original BCS mean-field theory may be relevant to topological properties predicted based on mean-field approximations. In fact, as we shall show in the next chapter by a case study, it is essential to include modification beyond BdG framework for gauge invariance to enforce physically correct result on Berry phase of transporting localized quasiparticles in a moving superconducting condensate. Here, we illustrate the issue by showing that the homogeneous BCS ground state wave function violates sum rule and how one might modify it, followed by an example in Section 3.1.2.1 in which a gauge invariant calculation taking proper account of condensate dynamics is essential.

The well-known homogenous BCS ground state wave function is given by

$$|\mathrm{GS}\rangle_{\mathrm{BCS}} = \prod_k (u_k + v_k a_k^\dagger a_{-k}^\dagger)|\mathrm{vac}\rangle, \tag{3.4}$$

where $u_k^2 = 1/2(1 + \epsilon_k/E_k)$ and $v_k^2 = 1/2(1 - \epsilon_k/E_k)$, ϵ_k is single particle kinetic energy defined relative to Fermi energy, $E_k = \sqrt{\epsilon_k^2 + \triangle^2}$ is quasiparticle energy spectrum. For simplicity, I have omitted spin indices. Let's evaluate long wavelength density fluctuations in the BCS ground state:

$$\lim_{q/k_F \to 0} \langle \rho_q \rho_{-q} \rangle \simeq 2\pi \triangle N(0), \tag{3.5}$$

where $N(0)$ is density of states at Fermi surface and $\triangle$ is superconducting gap. This can be calculated by expanding ρ_q and ρ_{-q} in terms of Bogoliubov quasiparticles $\alpha_{k\sigma}^\dagger$ with energy $E_{k\sigma} = \sqrt{\epsilon_k^2 + |\triangle|^2}$ and making use of $\langle \alpha_{k\sigma} \alpha_{k'\sigma'}^\dagger \rangle = \delta_{kk'} \delta_{\sigma\sigma'}$, $\langle \alpha_{k\sigma} \alpha_{k'\sigma'} \rangle = \langle \alpha_{k\sigma}^\dagger \alpha_{k'\sigma'}^\dagger \rangle = 0$. It is approaching a constant in the long wavelength limit, violating sum rules (f-sum rule and compressibility sum rule). We can see this as follows: the upper bound of long wavelength density fluctuation can be found from Cauchy-Schwartz inequality combined with f-sum rule and compressibility sum rule as

$$\lim_{q/k_F \to 0} \langle \rho_q \rho_{-q} \rangle < \frac{Nq}{mc}, \tag{3.6}$$

where N is total particle number and c is speed of low energy hydrodynamic mode which is of order Fermi velocity. So the long wavelength density fluctuation vanishes as q approaches zero.

We may modify the BCS ground state wave function by including hydrodynamic modes and write down the following ansatz

$$|\mathrm{GS}\rangle_{\mathrm{mod}} = \exp(-\sum_q \lambda_q \rho_q \rho_{-q})|\mathrm{GS}\rangle_{\mathrm{BCS}}, \tag{3.7}$$

where $\lambda_q = mc/(Nq)$.

In the above ansatz, long wavelength density fluctuations are damped by λ_q as q approaches zero.

3.1.2.1 An Example of Failure of Application of the BdG equations - NMR signature of ^{3}He-B Surface

Here we present an example where gauge invariant calculation taking into account superfluid condensate dynamics is essential in obtaining correct physics. We consider NMR longitudinal absorption in a ^{3}He-B film. It is well known that for a bulk ^{3}He-B, the longitudinal absorption is solely due to nuclear spin dipole interaction which is the only source in the Hamiltonian breaking rotation symmetry of spin relative to orbital and so resonance peak is completely determined by dipolar energy whose dominant contribution comes from the superfluid condensate spins due to their collective behavior (see e.g., [28] and [29], for a review, see [30]). Including the surface shouldn't qualitatively change the nature of NMR response. However, if we implement mean-field calculation as Silaev did [31], we will get qualitatively wrong signal in which absorption starts from the surface BdG quasiparticle energy gap which is dependent on the Larmour frequency. In particular, in the limit of vanishing external magnetic field, the absorption starts from zero frequency signaling the zero energy Majorana modes localized at the surfaces. In this example, we see that if condensate has interesting internal structure which is spin structure in this case, we need to pay attention to the condensate dynamics and shouldn't take for granted to regard condensate as c-number background. Technically, in this example, mean-field calculation based on BdG equations breaks conservation laws. A gauge invariant calculation (for gauge invariant schemes see e.g. [32]) has been done by Taylor et al. [33] and they confirmed that the qualitative feature of NMR absorption is unchanged from that of the bulk. See figure 3.1 for an illustration of NMR longitudinal absorption of a ^{3}He-B film.

3.1.3 Galilean Invariance

The lack of particle number conservation in the BCS theory also results in violation of Galilean invariance which we illustrate here by comparing the momentum of a BdG quasiparticle in two reference frames, one boosted from the other by a finite velocity. The BdG quasiparticle is created in a BCS s-wave uniform superfluid whose form is given in the standard form

$$\alpha_k^\dagger = u_k a_{k\uparrow}^\dagger + v_k a_{-k\downarrow}, \tag{3.8}$$

with the corresponding BCS ground state wave function taking the standard BCS form $|\mathrm{GS}\rangle = \prod_k (u_k - v_k^* a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger)|\mathrm{vac}\rangle$ in the lab frame. We first calculate in the lab frame the momentum of the quasiparticle described by (3.8) by comparing the total momentum of the superfluid with and without the quasiparticle excitation

$$p_{\mathrm{lab}} = \langle \alpha_k P \alpha_k^\dagger \rangle - \langle P \rangle = \langle \alpha_k, [P, \alpha_k^\dagger] \rangle. \tag{3.9}$$

The commutator of total momentum operator P with $\alpha_k^\dagger$ is evaluated to be $k\alpha_k^\dagger$. Inserting it back to the above equation, we get $p_{\mathrm{lab}} = k$. This is what we expect.

Now we boost the superfluid by switching to a moving frame in which the ground state wave function becomes $|\mathrm{GS}'\rangle = \prod_k (u_k - v_k^* a_{k+K/2\uparrow}^\dagger a_{-k+K/2\downarrow}^\dagger)|\mathrm{vac}\rangle$ with total momentum of each Cooper pair equal to K. The corresponding quasiparticle creation operator in the boosted superfluid is given by

$$\tilde{\alpha}^\dagger = u_k a_{k+K/2\uparrow}^\dagger + v_k a_{-k+K/2\downarrow}. \tag{3.10}$$

The quasiparticle momentum in the boosted frame is evaluated in a similar way to be

$$p_{\mathrm{boost}} = k + \frac{K}{2}(|u_k|^2 - |v_k|^2). \tag{3.11}$$

This result violates the Galilean invariance according to which we expect the quasiparticle momentum in the boosted frame to be $k + K/2$. This is simply due to particle number non-conserving form of the many-body wave functions. As we compare the expectation value of total particle number of many-body eigenstates with and without the quasiparticle excitation, the particle number is not increased by one, but by $|u_k|^2 - |v_k|^2$. Therefore in the boosted frame, the momentum change due to the quasiparticle is not equal to $k + K/2$. The resolution for fixing this problem is either to adjust coefficient of u_k and v_k for all k when the quasiparticle is added to the superfluid ground state to ensure average particle number is increased by one or simply to associate a Cooper pair creation operator to the hole part of the quasiparticle. If we associate a Cooper pair to the hole part of the quasiparticle, the boosted particle momentum satisfies Galilean invariance

$$\begin{aligned} p'_{\text{boost}} &= k + \frac{K}{2}(|u_k|^2 - |v_k|^2) + K|v_k|^2 \\ &= k + \frac{K}{2}(|u_k|^2 + |v_k|^2) = k + \frac{K}{2}, \end{aligned} \tag{3.12}$$

where the last term on rhs of first equality above is contribution from the Cooper pair to the momentum. This result satisfies Galilean invariance.

This simple example illustrates possible violation of fundamental physical principles due to particle number non-conserving in the standard mean-field approach. In this particular example, we see that extra care needs to be taken when the superfluid is moving.

3.2 Particle-Hole Symmetry

As discussed in Chapter 2, the particle-hole symmetry of BdG spectrum and BdG solutions plays a central role in deriving the reality condition of local bound states which in turn means Majorana modes. However, in physical particle number conserving systems, there's no exact particle-hole symmetry as hole is inequivalent to particle simply because they have different effect on total particle number. If the existence of Majorana zero modes necessarily depends on the particle-hole symmetry, then its very existence is questionable if there's no particle-hole symmetry. We'll speculate in Chapter 5 the possibility of local distinguishability due to different occupation of Majorana zero modes (or more precisely Dirac zero modes made out of them).

3.3 BdG Equations vs. Many-Body Energy Eigenstates

Finally, there is a very subtle point that hasn't been addressed so far. It's worth pointing it out here, though we didn't study it in this thesis. In all discussions so far, we have implicitly assumed that there exist many-body energy eigenstates corresponding to BdG equations. This is true under quite general conditions (see e.g., Appendix A in [34]), but is not guaranteed to be true. Solutions to BdG equations connect different many-body energy eigenstates, but there is no guarantee that there always exist such eigenstates that satisfy BdG equations. For an earlier discussion on such type of problems, see [35].

3.4 Figure

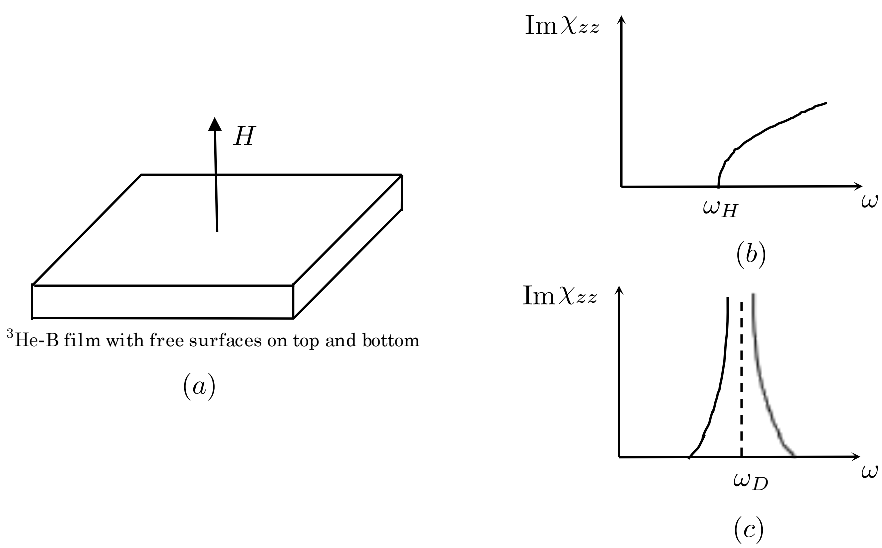

Figure 3.1: NMR longitudinal absorption of a ^{3}He-B film. (a) system setup, magnetic field H is uniform pointing in z direction (b) prediction based on mean-field BdG solutions: the absorption occurs at Larmour frequency ω_H (c) result based on gauge invariant calculation by Taylor et al.: the absorption signal agrees qualitatively with that of the bulk with resonance frequency determined by nuclear spin dipole energy ω_D broadened by Majorana zero modes at the film surface, sketch is adapted from figure 3 of [33].

Chapter 4

Berry Phase of Transporting a Localized Quasiparticle Around a Vortex in Superconductor

In this chapter, we start our investigation on effect of particle number conservation on topological properties of superconductors by studying the simplest case of Abelian phase, namely the Berry phase accumulated by a quasiparticle moving around an isolated Abrikosov vortex. As Berry phase of a localized quasiparticle moving around a vortex is a key physical quantity involved in determining braiding statistics of Majorana zero modes in vortices in topological superconductors, it's a good starting point to have a clear understanding of this basic process. We shall see that in our toy model, particle number conservation is necessary for ensuring a physical value of Berry phase and standard mean field approximation and BdG equations result in divergent result.

4.1 Model Setup

As we want to take into account the condensate to enforce particle number conservation, knowledge of Cooper pair wave function is presumably needed for calculating its contribution to the Berry phase since BdG quasiparticle itself being superposition of particle and hole, explicitly breaks particle number conservation and we need to associate a Cooper pair to the hole to recover particle number conservation. In the presence of a vortex, it is impractical to know the explicit form of Cooper pair wave function. So we make an assumption that it is only the topological feature of a vortex, namely its winding number, not its detailed structure, that determines the Berry phase. Therefore, we consider superfluid confined in annulus geometry with non-zero winding number of Cooper pair center-of-mass phase. The effective system is essentially one dimensional in azimuthal direction which greatly simplifies calculations. An external magnetic flux can be applied through the hole of the annulus to tune the superfluid velocity. We shall consider cases of both zero and non-zero superfluid velocity by tuning the flux. The latter case has useful applications in understanding physical constraints on braiding Majorana zero modes in two dimensional systems such as candidate topological superconductor Sr_2RuO_4 where penetration depth is much larger than coherence length so that the separation between vortices used for braiding may well be less than the penetration depth. When this happens, localized Majorana zero modes are immersed in superfluid with non-zero superfluid velocity due to the neighboring vortices. So studying the non-zero superfluid velocity has also practical importance.

In order to localize a quasiparticle, we need to apply some external potential to interact with it. At the same time, we want to keep its effect on the condensate as little as possible to simplify the many-body effect. To this end, we consider the simple BCS s-wave superconductor with odd total number of particles and we apply a weak localized Zeeman field whose spatial extension is much larger than the coherence length. To the first order in the Zeeman field strength, the condensate can be approximated as unaffected. Since the total particle number is odd, one quasiparticle with spin orientated along the direction of the Zeeman field is localized. We then adiabatically move the Zeeman field around the annulus and study the Berry phase in such a process (see figure 4.1 for an illustration of system setup). The detailed discussions on how to trap a localized quasiparticle and its microscopic description will be delayed to Section 4.3.3 when we actually need to consider microscopic details.

4.2 Standard Particle Number Non-Conserving Argument

In the standard mean-field approximations, particle number conservation is broken down to Z_2 symmetry. Intuitively, we may forget about the condensate and regard the system as an effective single particle with pseudo-spin degree of freedom representing particle and hole component. Making analogy of the BdG equation for the quasiparticle to a Schrodinger equation for a spin-1/2 in a magnetic field illustrated in figure 4.2, we can map the kinetic energy of particle and hole to z-component of the effective magnetic field and superconducting gap plays the role of the magnetic field in x-y plane. Namely, the BdG equation for the quasiparticle

$$\begin{pmatrix} H_\uparrow & \triangle(r) \\ \triangle^*(r) & -H_\downarrow \end{pmatrix} \begin{pmatrix} u_\uparrow(r) \\ v_\downarrow(r) \end{pmatrix} = E \begin{pmatrix} u_\uparrow(r) \\ v_\downarrow(r) \end{pmatrix}, \tag{4.1}$$

where $\triangle(r) = |\triangle| \mathrm{e}^{in\theta}$, can be identified with the Schrodinger equation of a spin in a rotating magnetic field

$$\begin{pmatrix} B_z & B(r) \\ B^*(r) & -B_z \end{pmatrix} \begin{pmatrix} s_\uparrow \\ s_\downarrow \end{pmatrix} = E \begin{pmatrix} s_\uparrow \\ s_\downarrow \end{pmatrix}. \tag{4.2}$$

As the quasiparticle is moved around the annulus and returned to its starting point, the local superconducting gap phase seen by the quasiparticle is winded by $2n\pi$ where n is the winding number of the vortex and so the effective magnetic field is rotated about z axis by $2n\pi$. For a bound state, the particle and hole component have the same weight (this can be seen as follows: the particle gets reflected back at the trap edge and becomes hole which later reflects back as particle; since the quasiparticle is trapped inside, the particle and hole must have the same weight: if we "observe" the quasiparticle, we have equal probability of finding it in particle and in hole state), so the effective spin lies in the x-y plane. From well known result of Berry phase of the spin 1/2 in the magnetic field, we immediately get the Berry phase to be $n\pi$ [36]. This result appears to be insensitive to whether there is magnetic flux through the annulus. I will discuss next calculations taking into account the full many-body wave function of the system and we will see that argument ignoring particle number conservation gives a different answer.

4.3 Particle Number Conserving Argument

In this effective 1d system, the Berry phase is given by the total angular momentum of the system. This is because we can write the many-body ground state of the system in the form $\Psi(\{\theta_i - \theta_0\})$, where only azimuthal coordinate is considered, θ_i is the coordinate of particle i which runs from 1 to $2N+1$ and θ_0 parameterizes the position of the Zeeman trap. The Berry phase can then be shown to be equal to total angular momentum of the system as follows

$$\begin{aligned}\phi &= -\mathrm{Im}\{\int_0^{2\pi} \langle\Psi|\frac{\partial\Psi}{\partial\theta_0}\rangle\} \\ &= \mathrm{Im}\{\sum_{i=1}^{2N+1}\int_0^{2\pi} \langle\Psi|\frac{\partial\Psi}{\partial\theta_i}\rangle\} \\ &= 2\pi\sum_{i=1}^{2N+1} L_i, \end{aligned} \tag{4.3}$$

where L_i denotes the expectation value of angular momentum of particle i.

It turns out that at integer magnetic fluxes (measured in unit of $h/2|e|$), we can find the angular momentum exactly based on general argument of gauge transformation and time reversal symmetry. Away from integer fluxes, the angular momentum can't be found exactly and we need to resort to linear order perturbation.

4.3.1 Integer Flux

The Hamiltonian is given by

$$H = \sum_{j=1}^{2N+1}(-i\frac{\partial}{\partial\theta_j}+\Phi)^2 + V_{\mathrm{int}} + H_z, \tag{4.4}$$

where V_{int} is particle particle interaction term, Φ is external magnetic flux in units of $h/|e|$ and H_z is Zeeman term. Making the gauge transformation to the 2N+1 wave function Ψ

$$\tilde{\Psi} = \exp(i\sum_{j=1}^{2N+1}\Phi\theta_i)\Psi \tag{4.5}$$

and substitute into the Schrodinger equation, we get

$$\tilde{H}\tilde{\Psi} = E\tilde{\Psi}, \tag{4.6}$$

where $\tilde{H} = -\sum_{j=1}^{2N+1} \partial^2/\partial\theta_j^2 + V + H_z$. The transformed many-body function satisfies the boundary condition

$$\tilde{\Psi}(\theta_i + 2\pi, ...) = \exp(i2\pi\Phi)\tilde{\Psi}(\theta_i, ...). \tag{4.7}$$

When $2\Phi = n$, the boundary condition (4.7) after the gauge transformation is invariant under time reversal. Since the transformed Hamiltonian $\tilde{H}$ also has time reversal symmetry (note that the Zeeman term is unchanged since the time reversal considered here is with respect to orbital degrees of freedom only), the ground state wave function $\tilde{\Psi}$ must be real if there is no degeneracy. So its angular momentum is zero. Thus, the angular momentum of the original wave function is

$$L = -\sum_{i=1}^{2N+1} \Phi = -(2N+1)\Phi. \tag{4.8}$$

Similarly for even number of particles, the angular momentum is $-2N\Phi$. Note that the above result (4.8) is very general and exact and furthermore doesn't depend on details of the system such as whether it's superconducting or not. It is also different from general theorem of Byers and Yang [37] in that it is a stronger statement on non-degenerate eigenstates at integer fluxes of $h/2|e|$, instead of $h/|e|$. It is rather interesting to see that the fluxes quantized at integer values of $h/2|e|$ are special in that the Berry phase of transporting any local potential (in the case of current interest, it is the Zeeman field) becomes just the sum of AB phase of each individual particle moving around the annulus. Usually, $h/2|e|$ is related to Cooper pairing. However, here it enters in quite general situations.

Equation (4.8) can be applied to our toy model when the superfluid velocity vanishes. Since at zero superfluid velocity, we have

$$l_0 + 2\Phi = 0, \tag{4.9}$$

where l_0 is the winding number of superconducting order parameter. For vortex winding number $l_0 = 1$, $\Phi = -1/2$ which is at integer value of $h/2|e|$. Furthermore, we know the ground state is unique for our system with a single bound quasiparticle in potential well (the energy from spin degree of freedom is split due to Zeeman field). According to (4.8) and (4.3), the Berry phase is equal to π. Thus the intuitive argument given above using BdG equations is correct at zero superfluid velocity.

4.3.2 Linear Response Theory - away from Integer Flux

Away from integer flux, the boundary condition (4.7) is no longer invariant under time reversal and the above argument ceases to be valid. In order to proceed, we can regard the deviation of magnetic flux from integer values as perturbation and apply first order perturbation theory to the problem. This is valid if the annulus is large enough so that flux change of order 1 is really a small perturbation to the system compared to total energy of the system.

To obtain Berry phase that characterizes the quasiparticle statistics, we should compare the difference in Berry phase for system with $2N+1$ and $2N$ particles. Taking this into account and writing the Berry phase in terms of deviation from the value from integer magnetic flux, we get the following expression for the Berry phase at magnetic flux $\Phi = -1/2 + \delta\Phi$ (from now on, we fix the superconducting order parameter winding number to be 1)

$$\phi/2\pi = (\langle J_{2N+1}\rangle_{\Phi=-\frac{1}{2}+\delta\Phi} - \langle J_{2N+1}\rangle_{\Phi=-\frac{1}{2}}) - (\langle J_{2N}\rangle_{\Phi=-\frac{1}{2}+\delta\Phi} - \langle J_{2N}\rangle_{\Phi=-\frac{1}{2}}) + \frac{1}{2}, \tag{4.10}$$

where $J \equiv \sum_j -i\partial/\partial\theta_j$. Note that I use notation J here to emphasize relation between Berry phase and current response to transverse vector field acting on superfluid due to magnetic flux Φ threading the annulus. J is just the total angular momentum of the system.

Now apply standard first order perturbation theory, the current J difference at flux Φ and at flux $-1/2$ is

$$\begin{aligned} \langle\tilde{0}|J|\tilde{0}\rangle - \langle 0|J|0\rangle &= (\sum_n a_n \langle 0|J|n\rangle + c.c.) \\ &= 2\sum_n \frac{|\langle 0|J|n\rangle|^2}{E_0 - E_n}\delta\Phi, \end{aligned} \tag{4.11}$$

where $|\tilde{0}\rangle$ refers to the ground state at flux $\Phi = -\frac{1}{2}+\delta\Phi$, $|0\rangle$ and $|n\rangle$ refer to ground state and excited eigenstates at flux $\Phi = -\frac{1}{2}$ with energies E_0 and E_n, respectively, $|\tilde{0}\rangle = |0\rangle + \sum_n a_n|n\rangle$. We omit the subscript of the current J, which would be added for discussing $2N$ and $2N+1$ cases separately.

Let's first discuss the $2N$ particle ground state. If we assume the $2N$ particle ground state at flux $\Phi = -\frac{1}{2} + \delta\Phi$ has rotation symmetry, which is true to first order of the Zeeman field, then the matrix element $\langle 0|J|n\rangle$ vanishes identically and hence the correction due to $\delta\Phi$ in equation (4.11). So we have $\langle J_{2N}\rangle_{\Phi=-\frac{1}{2}+\delta\Phi} - \langle J_{2N}\rangle_{\Phi=-\frac{1}{2}} = 0$. This result is simply the Meissner effect which implies that the current-current correlation here is the transverse one and superfluid condensate doesn't contribute to it. This is intuitively reasonable since the current is responding to magnetic vector potential as in the usual Meissner effect and analogously superfluid in a rotating container.

What about the ground state with $2N+1$ particles? In this case, the ground state no longer has rotation symmetry, so the matrix element in equation (4.11) is finite. The sum rule of the current-current correlation here is rather tricky since we are considering ground state with odd total number of particles and it's unclear what accounts for normal fluid which is responsible for transverse current-current correlation. We may rewrite the sum in equation (4.11) as

$$2\sum_n \frac{|\langle 0|J_{2N+1}|n\rangle|^2}{E_0 - E_n} = -i\frac{\langle 0|[X,H] + \frac{i}{2}|n\rangle\langle n|J_{2N+1}|0\rangle}{E_0 - E_n} - i\frac{\langle 0|J_{2N+1}|n\rangle\langle n|[X,H] + \frac{i}{2}|0\rangle}{E_0 - E_n}, \tag{4.12}$$

where H is Hamiltonian at flux $\Phi = -1/2$, $X = \sum_{i=1}^{2N+1}\theta_i$. The constant $i/2$ in the matrix element in equation (4.12) comes from the fact that the kinetic term for each particle i in H takes the form $(-i\frac{\partial}{\partial\theta_i} - \frac{1}{2})^2$. The first sum in equation (4.12) can be rewritten as

$$-i\frac{\langle 0|[X,H] + \frac{i}{2}|n\rangle\langle n|J_{2N+1}|0\rangle}{E_0 - E_n} = i\langle 0|X|n\rangle\langle n|J_{2N+1}|0\rangle. \tag{4.13}$$

Similarly, the second sum in equation (4.12) can be written as

$$-i\frac{\langle 0|J_{2N+1}|n\rangle\langle n|[X,H] + \frac{i}{2}|0\rangle}{E_0 - E_n} = -i\langle 0|J_{2N+1}|n\rangle\langle n|X|0\rangle. \tag{4.14}$$

Now, adding equation (4.13) and (4.14), together with a term $i\langle 0|X|0\rangle\langle 0|J_{2N+1}|0\rangle - i\langle 0|J_{2N+1}|0\rangle\langle 0|X|0\rangle$

(which is zero), we get

$$
\begin{aligned}
2\sum_n \frac{|\langle 0|J_{2N+1}|n\rangle|^2}{E_0-E_n} &= i\langle 0|[X, J_{2N+1}]|0\rangle \\
&= -(2N+1). \qquad (4.15)
\end{aligned}
$$

So the Berry phase is, combing equation (4.10) with equation (4.15) and (4.11)

$$
\phi/2\pi = -(2N+1)\delta\Phi + \frac{1}{2}. \qquad (4.16)
$$

However, this derivation can't distinguish the longitudinal current from the transverse one as intuitively we know the superfluid condensate can't contribute to the transverse current-current correlation. If we apply the same derivation to the $2N$ particle ground state, we would arrive at Berry phase change away from $\Phi = -1/2$ proportional to $2N$ which conflicts with earlier argument. Mathematically, we can't simply take the commutation relation in (4.15) to be that of $[x, p]$ as here X is compact that $X \equiv X + (2N+1)2m\pi$ for any integer m. We should regard the (magnitude of) right hand side of equation (4.15) as upper bound of the (magnitude of) sum on the left hand side. In the following, we'll make various attempts to estimate the sum. We'll see that standard BdG equations violate the upper bound given by the right hand side of (4.15) and it's necessary to modify the many-body wave function beyond the mean-field construction to restore particle number conservation.

4.3.3 Continuity Condition

So far we have not considered microscopies of the system and our analysis till now is quite general. To proceed and evaluate (4.11), we need to make some specific reference to the microscopic Hamiltonian and study properties such as the energy spectrum of the quasiparticle. We first notice that all terms in the sum in (4.11) are negative and so they all contribute to the sum constructively. Let's start by looking into the lowest energy state contribution to the sum which corresponds to bound quasiparticle states. For this, we need to explicitly consider wave functions and energy spectrum of the bound states. For simplicity, we restrict to the simplest case with zero superfluid winding number in the absence of magnetic flux. Straightforward generalizations to other cases will be given directly without explicit derivations.

We are considering $2N+1$-particle superconducting system whose condensate forms BCS s-wave Cooper pairing. In the absence of any external potential field, low energy eigenstate states in the BCS mean-field framework are approximated by $2N$-particle BCS ground state (particle-number conserving BCS ground state) added by a particle number conserving BdG quasiparticle

$$|\mathrm{GS}\rangle_{2N+1} = \alpha^{\dagger}_{k,\sigma}|\mathrm{GS}\rangle_{2N} \tag{4.17}$$

with

$$\alpha^{\dagger}_{k\sigma} = u_k a^{\dagger}_{k\sigma} + \sigma v_k a_{-k,-\sigma} C^{\dagger} \tag{4.18}$$

and

$$|\mathrm{GS}\rangle_{2N} = C^{\dagger N}|\mathrm{vac}\rangle, C^{\dagger} = \sum_k c_k a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow}, \tag{4.19}$$

where $|\mathrm{vac}\rangle$ denotes the particle vacuum state, $C^{\dagger}$ creates Cooper pairs in BCS ground state, and coefficients c_k are given by

$$c_k = v_k/u_k, \;\; u_k, v_k = \sqrt{1/2}(1 \pm \epsilon_k/E_k), \tag{4.20}$$

where $\epsilon_k = \hbar^2(k^2 - k_F^2)/2m$, $E_k = \sqrt{\epsilon_k^2 + |\bigtriangleup|^2}$, k_F is Fermi wave vector and $\bigtriangleup$ is the BCS energy gap. k near Fermi wave vector correspond to near gap excitations.

Adding a weak Zeeman field $B(z)$ as a function only of z (longitudinal direction along annulus), we get a Zeeman term in the Hamiltonian as

$$\sum_i \sigma_i V(z_i), \;\; V(z) = -\mu B(z), \tag{4.21}$$

where μ is magnetic moment of particles and σ_i is projection of spin along axis of B.

We consider regime of Zeeman field such that a BdG quasiparticle is trapped well within the Zeeman potential and at the same time the condensate can be considered as unaffected. So we require the extension of Zeeman field d to be much larger than the coherence length ξ and its strength V_0 much smaller than $\triangle$. To trap a quasiparticle within its extension, we require the kinetic energy cost inside the trap be smaller than binding energy, $\hbar v_F/d < V_0$, which is consistently satisfied by the previous requirement of $d \gg \xi$. Finally, the Zeeman field extension should be much smaller than the circumference of the annulus $L = 2\pi R$.

Let's choose the direction of the Zeeman field to be pointing up, so that the localized quasiparticle has spin up in lowest energy eigenstates. Due to the Zeeman term, Fourier components of BdG quasiparticle with different momenta will scatter into each other and we expect a bound quasiparticle to be formed out of linear combination of $\alpha^\dagger_{k\uparrow}$ with k around Fermi wave vector $\pm k_F$. Ignoring normal reflection, we can consider wave packet around either k_F or $-k_F$ and the resulting wave functions are described by Andreev bound states [38]. As bound quasiparticle states with wave vectors in $+z$ and $-z$ directions are degenerate, we can't use them to evaluate the sum in 4.11 which would result in divergence. So we have to take into full account of normal reflection which is usually ignored in discussion of Andreev problems. Although normal reflection splits the lowest two energy levels and avoids divergence, there's something wrong with the energy splitting as described by the BdG equations. For a smooth Zeeman trap varying at length scale much larger than the coherence length, the coupling due to normal reflection is exponentially small determined by the ratio of Zeeman length scale to inverse of Fermi wave number, i.e., it scales as $\exp(-k_F d)$. On the other hand, we can show that the numerator $|\langle 0|J|1\rangle|^2$ remains finite in the limit $d/\xi \to \infty$, yielding divergent contribution to the sum. This violation of sum rule is closely related to violation of continuity condition and corresponding particle number conservation in the mean-field approach. This is can be seen as follows. If the energy splitting of the doublet is exponentially small and suppose the quasiparticle is in the quasi-ground state with wave vector centered around Fermi wave vector k_F, then the state is quasi-stationary with lifetime of order the inverse of the exponentially small energy splitting. Now by continuity condition of particle flow, the divergence of particle number flow should be exponentially small everywhere in the annulus. But this is in contradiction to the corresponding many-body state. As the quasiparticle is localized inside the Zeeman trap, the current outside the trap is zero (remember that we are considering the state with vanishing superfluid velocity) and the current inside is of order v_F/d. So the divergence of current is much larger than required by continuity condition [39]. This suggests necessity of going beyond mean field BdG equations to enforce particle number conservation in order to satisfy the f-sum rule.

One of the reasons the BdG approach fails in the above analysis is neglecting the superconducting condensate and treating the system as an effective single particle problem associated with the quasiparticle that doesn't preserve particle number conservation. Hence we'll make a variational ansatz to the particle number conserving many-body ground state in order to recover continuity condition though systematic constructions of post-BdG formalism are lacking. To avoid finite current divergence at the edges of Zeeman trap for bound quasiparticle approximate energy eigenstate with wave vector around k_F, it's natural to imagine some counterflow from the superconducting condensate inside the trap to cancel the current flow induced by the bound quasiparticle. Although neither the condensate nor the quasiparticle satisfies continuity condition alone, the combination of the two as the whole satisfies the continuity condition. Energetically, the most economical way to generate superfluid flow is to twist the superfluid phase. Hence, it suffices to multiply the 2N-particle ground state wave function (the $2N+1$-particle wave function is obtained by acting particle number conserving quasiparticle operator on the $2N$-particle state) by a phase factor $\exp(-i\sum_j f(z_j))$ to yield zero current flow throughout the annulus, where [38]

$$f(z) = \frac{k_F L}{2N} \int |\Psi_{\text{Sch}}(z)|^2 dz, \tag{4.22}$$

where L is circumference of the annulus, $\Psi_{\text{Sch}}(z)$ is wave function to a Schrodinger equation derived from the BdG equation for the quasiparticle and is related to particle and hole component $u(z)$ and $v(z)$ via $u(z) \approx v(z) = \exp(ik_F z)\Psi_{\text{Sch}}(z)$ (z is coordinate along the annulus).

We see that in the modified state, the superfluid condensate is deformed in the region where the quasiparticle is localized. For the true energy ground state doublet, the quasiparticle wave function is linear combination of two approximate quasiparticle energy eigenstates with wave vectors centered around $\pm k_F$. Once the superfluid condensate deformation is taken into account, the quasiparticle wave function is entangled with the condensate, a new feature absent in the standard BdG approach.

At this point, it's appropriate to mention a related consequence of breaking continuity condition in the particle number non-conserving BdG approach in calculating the Berry phase in our toy model. As the Berry phase ϕ of transporting the quasiparticle can be found from the difference in the total angular momentum between $2N+1$ particle and $2N$ particle states, making use of continuity condition to deduce that in a 1d system, the current is uniform throughout the annulus for any energy eigenstate and writing the $2N+1$ particle ground state as the BdG quasiparticle operator $\alpha^\dagger$ acting on the $2N$ particle ground state, we can write the Berry phase in terms of commutator between current density operator and $\alpha^\dagger$ at any arbitrary position θ'

$$
\begin{aligned}
\phi/2\pi &= L(\langle \alpha(\tilde{J}(\theta')\alpha^\dagger\rangle - \langle \tilde{J}(\theta')\rangle) - \Phi \\
&= L(\langle \alpha[\tilde{J}(\theta'), \alpha^\dagger]\rangle) - \Phi,
\end{aligned}
\tag{4.23}
$$

where the magnetic flux Φ appears due to converting angular momentum density to current at θ by $\tilde{J}(\theta) = J(\theta) + \Phi\rho(\theta)/L$. In the particle number non-conserving form, $\alpha^\dagger = \int d\theta u(\theta)\Psi^\dagger(\theta) + v(\theta)\Psi(\theta)$ where $u(\theta)$ and $v(\theta)$ are particle and hole wave functions localized at Zeeman trap around θ_0. We can always choose θ' to be sufficiently far away from θ_0 such that $[\tilde{J}(\theta'), \alpha^\dagger] = 0$. So the Berry phase is just given by Aharonov-Bohm phase at all magnetic fluxes. This result is in conflict with the intuitive one obtained using spin analogy in Section 4.2 where the Berry phase is found to be independent of magnetic flux. In the above derivation, the key step is to make use of continuity condition to replace total current by local current. Although the continuity condition is satisfied in the BdG formalism for any energy eigenstate or at thermal equilibrium, its validity in those situations is justified under particle number non-conserving approximation. Meanwhile, we should keep in mind that the system under consideration should have fixed particle number to have a physically meaningful quantum phase associated with adiabatic evolution. So the Berry phase of $-\Phi$ obtained from (4.23) doesn't correspond to a quantum state with fixed particle number and may not correspond to a physical result. The unphysical result will be modified already at a naive level of restoring particle number conservation. Once we add a Cooper pair creation operator associated with the hole part of the BdG quasiparticle, the commutator $[\tilde{J}(\theta'), \alpha^\dagger]$ becomes finite throughout the annulus since the Cooper pair wave function is spread out along the annulus. Before closing this paragraph, it is worth noting that the whole discussion in this paragraph is based on independent quasiparticle approximation so that $2N+1$ particle eigenstate can be related to $2N$ particle eigenstate through a quasiparticle. We know from previous discussion of continuity condition that this approximation is no longer valid in our toy model. Hence to get a physical value of the Berry phase, we should really consider many-body wave functions beyond the BdG approximation and avoid using many-body wave functions directly constructed from individual quasiparticle states.

4.3.4 Lower Bound on Berry Phase Change away from Integer Flux

In this section, we estimate lower bound of Berry phase change away from integer magnetic flux, i.e., the sum in equation (4.11). We will do this by two different approaches and they give the sam form of lower bound that is independent of Zeeman trap strength. In the first approach, we apply Cauchy-Schwartz (CS) inequality to estimate lower bound of the sum in equation (4.11). We noticed in evaluating the sum in equation (4.12)-(4.15) that we want to avoid evaluating angular momentum in terms of azimuthal coordinates as they are subtle in annulus geometry. With this in mind, we apply CS inequality consecutively to obtain the following inequality

$$\begin{aligned}
\sum_n \frac{|\langle 0|J|n\rangle|^2}{E_n - E_0} &> \frac{(\sum_n |\langle 0|J|n\rangle|^2)^2}{\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)} \\
&> \frac{(\sum_n |\langle 0|J|n\rangle|^2)^2}{\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)^2} \sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)^3 \\
&= \frac{(\sum_n |\langle 0|J|n\rangle|^2)^2 \sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)^2}{(\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)^2)^2} \sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)^3 \\
&> \frac{(\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0))^2 \sum_n |\langle 0|J|n\rangle|^2}{(\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)^2)^2} \frac{(\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)^2)^2}{\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)} \\
&> \frac{\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)}{(\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0)^2)^2} (\sum_n |\langle 0|J|n\rangle|^2 (E_n - E_0))^2 \\
&= -\frac{\langle [J,[J,H]]\rangle^3}{\langle [J,H]^2\rangle^2}. \qquad (4.24)
\end{aligned}$$

Evaluating $[J, H]$, we get

$$[J, H] = -iR \int_0^L ds \rho_{\sigma_z}(s) \partial/\partial_s V(s) ds, \tag{4.25}$$

where R is radius of annulus, $L = 2\pi R$ is circumference of annulus, $V_z(s)$ is Zeeman field, $\rho_{\sigma_z}(s)$ is spin density in $+z$ direction in which Zeeman field is oriented.

For wide and weak Zeeman field, we expect a net spin up to be localized in the trap. If we model the bottom of the trap by a Harmonic oscillator, $[J, H]$ becomes

$$[J, H] = -iRk \int drrS(r), \tag{4.26}$$

where I have used $S(r)$ to represent the localized spin density, k is strength of the oscillator. The denominator of rhs of equation (4.24) can be easily evaluated for a particle in a Harmonic oscillator to be

$$\langle [J, H]^2 \rangle^2 = \frac{k^3 R^4}{4m^*}, \tag{4.27}$$

where m^* is the effective mass. To obtain the effective mass, we need to explicitly write down the BdG equation for the localized quasiparticle which will be done shortly in the second approach. For now, we just quote the value $m^* = \frac{\triangle}{2\epsilon_F} m$ with m the bare particle mass, $\triangle$ is superconducting gap and ϵ_F is Fermi energy. $[J, [J, H]]$ is evaluated from (4.26) to be

$$[J, [J, H]] = -R^2 k \int drS(r) = -R^2 k, \tag{4.28}$$

where normalization condition $\int drS(r) = 1$ has been used.

Substituting (4.26) and (4.28) into (4.24) we obtain the lower bound

$$\sum_n \frac{|\langle 0|J|n\rangle|^2}{E_n - E_0} > 4R^2 m^*. \tag{4.29}$$

Taking into account units, the rhs of (4.29) becomes $4m^*/m = 2\triangle/\epsilon_F$. Hence, we see that the deviation of Berry phase away from integer magnetic flux has lower bound $-(4\triangle/\epsilon_F)\delta\Phi$ (keep in mind another factor of two in the sum 4.11).

Now, let's evaluate the lower bound directly from the BdG equation for the bound quasiparticle. Assuming $2N$-particle ground state wave function is unchanged by the Zeeman trap, we can write down the effective equation obeyed by the bound quasiparticle

$$E_k C_k - \sum_{k'} V_{k-k'} C_{k'} = E C_k, \tag{4.30}$$

where $V_{k-k'}$ is Fourier component of Zeeman trap and the bound quasiparticle state is given by linear superposition of plane wave quasiparticle states as

$$\alpha^\dagger = \sum_k C_k \alpha^\dagger_{k\uparrow}. \tag{4.31}$$

Expanding the excitation energy $E_k = \sqrt{\epsilon_k^2 + \triangle^2}$ to lowest order in $\epsilon/\triangle$ and considering wave numbers around $\pm k_F$, we get effective time independent Schrodinger equation obeyed by the bound quasiparticle with wave numbers in either direction

$$\frac{1}{2m^*}\frac{d^2}{dz^2} f(z) - V(z) f(z) = E f(z), \tag{4.32}$$

where effective mass is $m^* = (\triangle/2\epsilon_F)m$, $e^{i\pm k_F z} f(z) = \sum_{k,\pm k_F} C_k \exp ikz$ (the sum over k is near either k_F or $-k_F$).

When the superfluid has non-zero winding number around the annulus and also in the presence of finite magnetic flux, the effective equation given by (4.30) can be generalized by replacing momentum quantum number by angular momentum quantum number and the excitation energy becomes

$$E_l = \sqrt{\epsilon_l^2 + \triangle^2} + (l_0 + 2\Phi)(l - \frac{l_0}{2}), \tag{4.33}$$

where l_0 is winding number, Φ is magnetic flux and $\epsilon_l = (l - \frac{l_0}{2})^2 - \mu$.

If we ignore mixing of wave number from around k_F and around $-k_F$, the effective equation is again given by (4.32) but in the presence of effective vector potential. Minimizing kinetic energy, we obtain the average angular momentum

$$\langle l \rangle = l_{F\pm} - (l_0 + 2\Phi)\frac{\triangle}{2\epsilon_F}, \tag{4.34}$$

where $l_0 + 2\Phi$ is superfluid velocity, due to finite l_0, $l_{F+} + l_{F-} = l_0$ ($l_{F\pm}$ refer to positive and negative angular momentum at Fermi level respectively).

The Berry phase can be straightforwardly shown (by similar argument for the general case leading to equation 4.3, i.e., the bound quasiparticle wave function depends on Zeeman trap location parameterized by θ_0, so Berry phase is related to its angular momentum) to be equal to average angular momentum of the bound quasiparticle

$$\phi/2\pi = \langle l \rangle. \tag{4.35}$$

Ignoring redistribution of magnitudes of C_l around l_{F+} relative to those around l_{F-} due to magnetic flux change, we get a lower bound for the Berry phase change due to $\delta\Phi = \frac{1}{2} + \Phi$ (we specify the case of $l_0 = 1$ here)

$$\delta\phi/2\pi < -(\triangle/\epsilon_F)\delta\Phi \tag{4.36}$$

for positive $\delta\Phi$. Hence, we see that two approaches give the similar lower bound and the former approach gives a stronger bound (four times that of the latter bound).

In the second approach, we further see that the redistribution weights of C_l around positive and negative Fermi momentum due to finite superfluid velocity (i.e. finite $l_0 + 2\Phi$) is dependent on potential energy saving by scattering between opposite Fermi momenta through Zeeman trap (without the trap, all coefficients will be around either positive or negative Fermi momentum depending on sign of superfluid velocity). So for many-body wave functions constructed by BdG solutions, the Berry phase at general magnetic flux is non-universal and depends on parameters of the system such as Zeeman trap strength.

4.4 Berry Phase for the case of a Square Well Zeeman Trap

In this section, we evaluate the Berry phase quantitatively for a specific shape of Zeeman trap, a square well trap. We develop a different approach for calculating the Berry phase based on work-energy relationship. The advantage of this approach is that the Berry phase can be evaluated from energy of bound quasiparticle which is addressed by the BdG equations, without the need to explicitly referring to quantities more difficult to calculate such as angular momentum and many-body wave functions.

We have shown from symmetry that the Berry phase is π (equal to the AB phase) at magnetic flux $\Phi = -\frac{1}{2}$ (in unit of $h/|e|$) and vanishing superfluid velocity $v_s \propto l_0 + 2\Phi = 0$ (l_0 is the winding number of pair wave function). We are interested in knowing the evolution of the Berry phase as we change the magnetic flux while keeping the winding number l_0 fixed. As we change the magnetic flux, a voltage is generated along the ring. The amount of work done to the system is determined by the voltage and the current. Since work is equal to energy change, we can establish a relationship between the Berry phase (through current) and variation of quasiparticle energy.

The work-energy equations for the system with $2N$ and $2N+1$ particles are

$$\begin{aligned}
\int_{\Phi_i}^{\Phi_f} (L_{2N} + 2N\Phi) d\Phi &= E_{2N}(\Phi_f) - E_{2N}(\Phi_i) \\
\int_{\Phi_i}^{\Phi_f} (L_{2N+1} + (2N+1)\Phi) d\Phi &= E_{2N+1}(\Phi_f) - E_{2N+1}(\Phi_i),
\end{aligned} \tag{4.37}$$

where L denotes total angular momentum, E refers to total energy of the system and Φ is external magnetic flux. All three quantities are dimensionless with units $\hbar$, $\hbar^2/2mR^2$ (R - annulus radius) and $h/|e|$, respectively. Subtracting the two equations, we obtain

$$\int_{\Phi_i}^{\Phi_f} (L_{2N+1} - L_{2N} + \Phi) d\Phi = (E_{2N+1}(\Phi_f) - E_{2N}(\Phi_f)) - (E_{2N+1}(\Phi_i) - E_{2N+1}(\Phi_i)). \quad (4.38)$$

Differentiating equation (4.38), we get

$$L_{2N+1} - L_{2N} = -\Phi + dE(\Phi)/d\Phi, \quad (4.39)$$

where $E(\Phi) \equiv E_{2N+1}(\Phi) - E_{2N}(\Phi)$ is the quasiparticle energy.

Since the Berry phase ϕ is equal to $2\pi L$, we get the Berry phase from (4.39)

$$\phi/2\pi = -\Phi + dE(\Phi)/d\Phi. \quad (4.40)$$

The first term on rhs of equation (4.40) is just AB phase, the second term is correction due to energy dependence on magnetic flux.

We now solve BdG equations to find $E(\Phi)$. In order to find a simple analytic expression, we choose a square shaped Zeeman trap, i.e. it is constant between $\theta = -\theta_L/2$ and $\theta = \theta_L/2$ and zero elsewhere. We also ignore any spatial inhomogeneity of the gap magnitude.

We consider magnetic flux around $-1/2$, where the BdG equation reads

$$\begin{aligned} ((l - \frac{1}{2})^2 - \mu) u + \triangle e^{i\theta} v &= (E + V) u \\ -((l + \frac{1}{2})^2 - \mu) v + \triangle e^{-i\theta} u &= (E + V) v, \end{aligned} \quad (4.41)$$

where V is the Zeeman potential, it's zero between θ_L and 2π and equal to V outside. $\triangle$ is constant to a good approximation and it can be made to be real, l is angular momentum quantum number, μ is chemical potential. Let's make the gauge transformation $u = \tilde{u} e^{i\theta/2}$, $v = \tilde{v} e^{-i\theta/2}$. After the transformation and rename $\tilde{u}$, $\tilde{v}$ to u, v, we get

$$\begin{aligned} (l^2-\mu)u+\triangle v &= (E+V)u \\ -(l^2-\mu)v+\triangle u &= (E+V)v. \end{aligned} \tag{4.42}$$

Now u and v are anti-periodic.

When the magnetic flux is $\Phi = -\frac{1}{2}+\lambda$, the BdG equation becomes

$$\begin{aligned} ((l+\lambda)^2-\mu)u+\triangle v &= (E+B)u \\ -((l-\lambda)^2-\mu)v+\triangle u &= (E+B)v, \end{aligned} \tag{4.43}$$

where again u and v satisfy anti-periodic boundary condition. The BdG equation (4.43) has the following symmetry: $\lambda \to -\lambda$, $E \to E$ for $(u,v) \to (u^*, v^*)$. Thus, the lowest energy eigenvalue $E_0(\lambda)$ is symmetric around $\lambda = 0$. So $dE(\Phi)/d\Phi = 0$ at $\Phi = -1/2$, and equation (4.40) gives just AB phase at $\Phi = -1/2$, consistent with previous general consideration based on symmetry (cf. Section 4.3.1).

If we ignore mixing between positive and negative momenta, it's relatively straightforward to show that the lowest energy doublet is degenerate at $\Phi = -1/2$ and they are linear in λ with slope $\pm 2l_F$ ($l_F^2 = \mu$) (see appendix B for a detailed derivation). When mixing is taken into account, a energy gap is opened up at crossing point and we can write down energy spectrum for small λ as

$$E(\lambda) = \pm\sqrt{(2l_F\lambda)^2+\eta^2}, \tag{4.44}$$

where η is energy gap at $\Phi = -1/2$. So the lowest energy derivative with respect to λ is

$$dE/d\lambda = -4l_F^2\lambda/\sqrt{(2l_F\lambda)^2+\eta^2}. \tag{4.45}$$

It is interesting to note the follow points concerning (4.45). Firstly, it satisfies f-sum rule and its upper bound is just half of the upper bound of f-sum rule for a true 1D system since the magnitude of the rhs is bounded by $2l_F$ which is equal to total number of particles for each spin. For physical system of interest, the system is only quasi-1D and therefore the upper bound is smaller than half the upper bound of f-sum rule. Secondly, when comparing (4.45) with (4.11), we see that in the linear regime where $2l_F\lambda \ll \eta$, the Berry phase for a square well takes the same form as the doublet contribution to the sum in the linear response formula (up to a factor of 2) at BdG level (i.e., many-body deformation is not taken into account).

4.5 Summary

We see in this chapter that the Berry phase of transporting a quasiparticle around a vortex is a rather subtle problem. At the most naive level, we can regard the bound quasiparticle as single particle problem and map it into effective spin 1/2 in magnetic field. The Berry phase is found to be equal to π irrespective of external magnetic flux through the annulus (Section 4.2). Noticing that the Berry phase can be related to total angular momentum of the system in one dimension and making use of continuity condition, the Berry phase can be obtained by evaluating commutation relation between localized quasiparticle operator and local current operator (4.3.3). In the standard particle number non-conserving formalism, the commutator vanishes as Cooper pair operator associated with hole part of the quasiparticle is neglected. Therefore, we obtain the Berry phase to be equal to AB phase at any magnetic flux. This conclusion is in contradiction with that obtained from effective spin model away from integer flux (in unit of $h/2|e|$).

At this stage, we see that even in the same particle number non-conserving approximation, different treatment could yield different result. At integer magnetic flux, symmetry argument yield exact result of the Berry phase to be equal to AB phase, a result independent of any approximation (Section 4.3.1). We see that the Berry phase from both approaches above in particle number non-conserving approximation is consistent with this general result. So the remaining question is what is the Berry phase away from integer flux.

To address this question, we need to explicitly take into account particle number conservation. From linear response theory (or alternatively, from adiabatic perturbation theory in a rotating frame in which the Zeeman trap is at rest), we can write the Berry phase in the sum given by equation (4.11). This sum puts a upper bound to the Berry phase to be equal to total number of particles of the system, i.e., $2N + 1$. An examination of the first term in the sum shows that it violates the upper bound as the energy splitting between lowest two energy levels is exponentially small for a wide smooth Zeeman trap. This violation is closely related to the violation of continuity condition for approximate eigenstates made out of linear combination of the doublet eigenstates, i.e, for approximate states traveling to either directions inside the trap. To resolve this issue, we propose to modify the condensate wave function in response to quasiparticles traveling in either directions such that the quasiparticle wave function and the condensate wave function is entangled (Section 4.3.3).

As it is necessary to consider many-body wave functions beyond BdG formalism in order to evaluate the sum in equation (4.11), it becomes very difficult to do so in practice. So we turn to estimating the sum by evaluating its lower bound. From both CS inequality and directly evaluating the quasiparticle wave function as solution to effective time independent Schrodinger equation, we get the same lower bound $2\triangle/\epsilon_F$. This lower bound rules out the Berry phase of π given by the effective spin model. Furthermore, in evaluating the quasiparticle wave function, we see that the Berry phase is non-universal depending on parameters of the system. Of course, this conclusion is based on many-body wave function constructed from BdG solutions and its validity beyond BdG approximation is not completely clear.

Finally, we explicitly calculate the Berry phase for a square well Zeeman trap by evaluating the energy derivative of quasiparticle with respect to magnetic flux. We again obtain a non-universal result similar to the contribution of doublet to the sum in (4.11) within BdG formalism. It's tempting to believe that the non-universality of the Berry phase at general magnetic flux is valid even beyond BdG approximations since we don't expect energy spectrum to modify significantly beyond the BdG equations.

Despite still lack of model independent result (in particular, independent of BdG equations) on the quantitative value of Berry phase, we hope to have convinced the reader through this chapter that careful treatment of BdG equations is needed regarding evaluating Berry phase and formalism beyond BdG framework may be necessary for obtaining physically correct result.

4.6 Figures

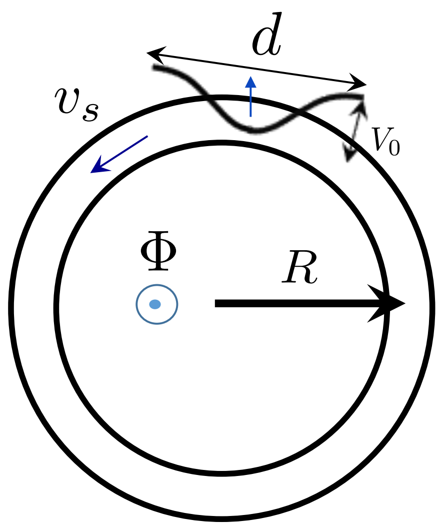

Figure 4.1: A bound quasiparticle with spin pointed along the direction of Zeeman field is formed in s-wave superfluid with odd number of particles confined in annulus geometry. d is spatial extension of Zeeman field, V_0 is its characteristic strength and superfluid velocity is given by $v_s = (n+2\Phi)h/2mR$, where Φ is magnetic flux through annulus in unit of $h/2|e|$, R is radius of annulus.

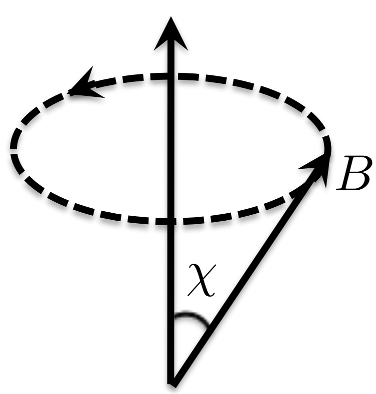

Figure 4.2: A bound quasiparticle as effective spin in magnetic field. For the bound quasiparticle, effective $\chi = \pi/2$, and Berry phase is $\phi = 2n\pi\cos^2(\chi/2) = n\pi$.

Chapter 5

Braiding Vortices in Chiral P-wave Superconductors

Having achieved some intuitive understanding of physics brought by particle number conservation and superconducting condensate in the toy model, we are ready to consider braiding Majorana zero modes in 2d superconducting systems and to explore consequences of particle number conservation and many-body wave function modifications beyond BdG approximations in braiding statistics and in topological properties in chiral p-wave superconductors. We will start in Section 5.1 by discussing general structure of degenerate ground state wave functions in ground state Hilbert subspace spanned by Majorana zero modes before focusing on Majorana zero modes localized in Abrikosov vortices in chiral p-wave superconductors. In Section 5.2, we will discuss effect of Cooper pair on braiding phases with two and four vortices at the level of mean-field BdG description but with fixed total number of particles. Finally in Section 5.3, we go beyond mean-field level and speculate the possibility of qualitative effect on topological property by superconducting condensate response to localize Majorana zero modes owing to particle number conservation.

5.1 Structure of Degenerate Ground State Wave Functions

We discuss structure of doubly degenerate ground states that are related to each other by two Bogoliubov Dirac-zero energy modes, or equivalently four Majorana zero modes. The doubly degenerate ground states constitute a basic qubit for quantum computing. In the standard picture, as we braid these Majorana zero modes, states undergo unitary evolution in the ground state subspace and we can effectively view the two ground states forming a Bloch spin 1/2 which rotates under braiding operation. We want to first ask whether it is possible to visualize the structure of the effective Bloch spin by relating its spin components to the underlying many-body ground state wave functions. This is motivated by well known Anderson pseudo-spin picture [11] of superconductors and the associated observation that in translational invariant superconducting eigenstates with even parity of particle number, excited eigenstates can be obtained from ground state by flipping pseudo-spins that are made of Cooper pair in momentum space. It is interesting to inquire whether this can be generalized to systems hosting Majorana zero modes. If this turns out to be true, then we will have a very simple physical picture relating two doubly degenerate ground states in which they are related to each other by flipping the Cooper pair component that comprises the Bloch spin. We perform our analysis within the mean-field BdG approximation in the standard particle number non-conserving form. The result can be easily generalized to particle number conserving case by projecting onto particle number basis.

In order to explore possible structure analogous to Anderson pseudo-spin picture, suppose we can write many-body ground states in Yang's form [40] (in the sense that Cooper pair wave function can be diagonalized) as follows

$$\begin{aligned} |00\rangle &= {\prod_n}' (u_n + v_n a_n^\dagger a_{\bar{n}}^\dagger)|\mathrm{vac}\rangle \\ |11\rangle &= (v_0 - u_0 a_0^\dagger a_{\bar{0}}^\dagger) {\prod_{n\neq 0}}' (u_n + v_n a_n^\dagger a_{\bar{n}}^\dagger)|\mathrm{vac}\rangle, \end{aligned} \tag{5.1}$$

where $a_n^\dagger$ and $a_{\bar{n}}^\dagger$ create single fermion states in vacuum that together form an orthonormal basis and prime superscripts over products are used to denote that sum is over half of all single particle states, i.e., only over states n, not $\bar{n}$ (states in the set of n and the set of $\bar{n}$ are mutually orthogonal) to avoid double-counting, since $a_n^\dagger a_{\bar{n}}^\dagger$ is the same as $a_{\bar{n}}^\dagger a_n^\dagger$ differing in a minus sign coming from Fermi statistics. The doubly degenerate ground states $|00\rangle$ and $|11\rangle$ are written in BCS form and we assume one pair associated with single particle state labeled by 0 and $\bar{0}$ are flipped. I have taken all u_n and v_n to be real and absorb all phases into single particle states.

In the BdG formalism, we know that $|11\rangle$ can be obtained from $|00\rangle$ by adding two zero energy BdG Dirac quasiparticles $\alpha_0^{00\dagger}$ and $\alpha_{\bar{0}}^{00\dagger}$ [41]

$$|11\rangle = \alpha_{\bar{0}}^{00\dagger}\alpha_0^{00\dagger}|00\rangle. \tag{5.2}$$

Let's express zero energy BdG quasiparticle states in terms of many-body ground state wave functions, i.e., in terms of u_n, v_n, $a_n^\dagger$ and $a_{\bar{n}}^\dagger$. From the requirement that a BdG quasiparticle annihilation operator must annihilate ground state, say $|00\rangle$ in this case, we can write down the most general form for the two zero energy BdG quasiparticle states as

$$\begin{aligned} \alpha_0^{00\dagger} &= \sum_n d_{0,n}(u_n a_n^\dagger + v_{\bar{n}} a_{\bar{n}}) \\ \alpha_{\bar{0}}^{00\dagger} &= \sum_n d_{\bar{0},n}(u_n a_n^\dagger + v_{\bar{n}} a_{\bar{n}}), \end{aligned} \tag{5.3}$$

where n run over all n and $\bar{n}$ corresponding to single particle states $a_n^\dagger$ and $a_{\bar{n}}^\dagger$ and $u_{\bar{n}} = u_n$, $v_{\bar{n}} = -v_n$.

From the requirement given by equation (5.2), we have the following constraint on coefficients $d_{0,n}$ and $d_{\bar{0},n}$

$$d_{0,\bar{0}} d_{\bar{0},0} - d_{0,0} d_{\bar{0},\bar{0}} = 1 \tag{5.4}$$

and all other d_n vanish.

From constraint (5.4), we can define another set of zero energy BdG quasiparticle operators as follows

$$\begin{aligned} \tilde{\alpha}_0^{00\dagger} &= u_0 a_0^\dagger - v_0 a_{\bar{0}} \\ \tilde{\alpha}_{\bar{0}}^{00\dagger} &= u_0 a_0^\dagger + v_0 a_{\bar{0}}, \end{aligned} \tag{5.5}$$

which are obtained from the original set of zero energy BdG quasiparticle operators by a unitary transformation.

For later comparison, we rewrite the new set of operators in terms of single particle wave functions $\phi_n(r)$ and $\phi_{\bar{n}}(r)$ which are created by $a_n^\dagger$ and $a_{\bar{n}}^\dagger$

$$\begin{aligned}
\tilde{\alpha}_0^{00\dagger} &= \int dr u_0 \phi_0(r)\psi^\dagger(r) - v_0\phi_{\bar{0}}^*(r)\psi(r) \\
\tilde{\alpha}_{\bar{0}}^{00\dagger} &= \int dr u_0 \phi_{\bar{0}}(r)\psi^\dagger(r) + v_0\phi_0^*(r)\psi(r).
\end{aligned} \tag{5.6}$$

On the other hand, we can write the above set of operators in linear combination of Majorana zero modes γ_i which are localized at four separate places r_i, $i = 1, \cdots, 4$ (for instance, sitting at four vortices) as

$$\begin{aligned}
\tilde{\alpha}_0^{00\dagger} &= \sum_{i=1}^{4} c_{0i} \int dr u_i(r)\psi^\dagger(r) + u_i^*(r)\psi(r) \\
\tilde{\alpha}_{\bar{0}}^{00\dagger} &= \sum_{i=1}^{4} c_{\bar{0}i} \int dr u_i(r)\psi^\dagger(r) + u_i^*(r)\psi(r),
\end{aligned} \tag{5.7}$$

where each MZM i is given by $\gamma_i = \int dr u_i(r)\psi^\dagger(r) + u_i^*(r)\psi(r)$ with field operator $\psi^\dagger(r)$ creating a particle at r.

Comparing wave functions given by equation (5.7) and (5.6), we get the following equations

$$\begin{aligned}
\frac{\sum_i c_{0i}^* u_i(r)}{\sum_i c_{\bar{0}i} u_i(r)} &= -\frac{v_0}{u_0} \\
\frac{\sum_i c_{0i} u_i(r)}{\sum_i c_{\bar{0}i}^* u_i(r)} &= \frac{u_0}{v_0}.
\end{aligned} \tag{5.8}$$

Since $u_i(r)$ is localized at position r_i, the above set of equations are satisfied iff

$$\begin{aligned}
\frac{c_{0i}^*}{c_{\bar{0}i}} &= -\frac{v_0}{u_0} \\
\frac{c_{0i}}{c_{\bar{0}i}^*} &= \frac{u_0}{v_0}
\end{aligned} \tag{5.9}$$

for each $i = 1, \cdots, 4$. (Equation 5.9 is necessary condition for 5.8 since near each Majorana zero mode, the left hand side in 5.8 becomes the left hand side in 5.9.)

However, there is no solution to (5.9). Thus, we see that it is not possible to find such a set of doubly degenerate ground states that admit simple relation between them by flipping one pair in Yang's form.

Since we are unable to find a simple relation between the doubly degenerate ground states in Yang's form, we next seek their structure relationship in terms of BdG solutions. It has been discussed in the work of Stern et al. [42] and they found that degenerate ground states are coherent superposition of states in which core states corresponding to local Majorana wave functions are either occupied or empty with equal weight. We give here a simple derivation for the cases of two and four Majorana zero modes which yield wave functions consistent with Stern et al's.

Consider two Majorana zero modes γ_1 and γ_2 described by localized wave functions as $\gamma_1 = a_1^\dagger + a_1$ and $\gamma_2 = a_2^\dagger + a_2$ with $a_1^\dagger$ and $a_2^\dagger$ creating localized wave functions at places r_1 and r_2. Define even particle number parity ground state $|0\rangle$ to be annihilated by $\alpha_0 = \gamma_1 - i\gamma_2$ and so odd particle number parity ground state is obtained from $|0\rangle$ by $|1\rangle = \alpha_0^\dagger|0\rangle$. From this definition, we can write down $|0\rangle$ and $|1\rangle$ in terms of $a_1^\dagger$ and $a_2^\dagger$ as

$$\begin{aligned} |0\rangle &= K(1 + ia_1^\dagger a_2^\dagger)|\Psi_\mathrm{e}\rangle + Q(a_1^\dagger - ia_2^\dagger)|\Psi_\mathrm{o}\rangle \\ |1\rangle &= K(a_1^\dagger + ia_2^\dagger)|\Psi_\mathrm{e}\rangle + Q(1 - ia_1^\dagger a_2^\dagger)|\Psi_\mathrm{o}\rangle, \end{aligned} \tag{5.10}$$

where K and Q are coefficients, $|\Psi_\mathrm{e}\rangle$ and $|\Psi_\mathrm{o}\rangle$ are many-body states with even and odd particle numbers respectively and neither of them contain single particle states associated with $a_1^\dagger$ and $a_2^\dagger$ (in the sense that we can expand $|\Psi_\mathrm{e}\rangle$ and $|\Psi_\mathrm{o}\rangle$ in products of single particle states which are all orthogonal to states associated with $a_1^\dagger$ and $a_2^\dagger$). We see from equation (5.10) that occupation of states $a_1^\dagger$ and $a_2^\dagger$ is of equal weight in both doubly degenerate ground states.

We can similarly write down doubly degenerate ground states with same particle number parity in terms of four Majorana zero mode wave functions $\gamma_i = a_i^\dagger + a_i$ $(i = 1, \cdots, 4)$. Define the two ground states by $|00\rangle$ and $|11\rangle = \alpha_{12}^\dagger \alpha_{34}^\dagger |00\rangle$ with $\alpha_{12}^\dagger = \gamma_1 + i\gamma_2$ and $\alpha_{34}^\dagger = \gamma_3 + i\gamma_4$. By requiring

$|00\rangle$ be annihilated by α_{12} and α_{34}, we find similar structure related to localized states

$$\begin{aligned}|00\rangle &= \lambda_1(1+ia_1^\dagger a_2^\dagger+ia_3^\dagger a_4^\dagger-a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger)|\Psi_{\rm e}\rangle+\lambda_2(ia_1^\dagger a_3^\dagger+a_1^\dagger a_4^\dagger+a_2^\dagger a_3^\dagger-ia_2^\dagger a_4^\dagger)|\Psi_{\rm e'}\rangle\\ &+ P_1(a_1^\dagger-ia_2^\dagger+ia_1^\dagger a_3^\dagger a_4^\dagger+a_2^\dagger a_3^\dagger a_4^\dagger)|\Psi_{\rm o}\rangle+P_2(ia_3^\dagger+a_4^\dagger-a_1^\dagger a_2^\dagger a_3^\dagger+ia_1^\dagger a_2^\dagger a_4^\dagger)|\Psi_{\rm o'}\rangle. \quad (5.11)\end{aligned}$$

5.2 Role of Cooper Pair in braiding MZM

In this section, we discuss braiding Majorana zero modes in systems with fixed particle number. We'll still consider many-body wave functions constructed from BdG solutions but with fixed particle number. Many-body states considered here with fixed particle number are the same as projected from particle number non-conserving states onto particle number sectors. To be more specific, take for example doubly degenerate ground states considered in Section 2.6 and write them out in terms of particle number basis

$$\begin{aligned}|0\rangle &= \sum_n A_n\Psi_{2n}\\ |1\rangle &= \sum_n B_n\Psi_{2n+1}, \end{aligned} \quad (5.12)$$

where Ψ_{2n} and Ψ_{2n+1} are normalized wave functions with $2n$ and $2n+1$ particles respectively. We are considering Berry phases of Ψ_{2n} and Ψ_{2n+1} with fixed n as we adiabatically braid (interchange in our discussion) two vortices. The Berry phase discussed in Section 2.6 in particle number non-conserving case is average Berry phase over states with different particle numbers (over all even particle numbers for $|0\rangle$ and odd particle numbers for $|1\rangle$).

There are some delicate points worthing clarifying before we start calculations for fixed particle number states. The first issue is concerned with total particle number. In the particle number non-conserving approximation, the two degenerate ground states that are related by two Majorana zero modes (and equivalently one Dirac zero mode) have the same average particle number which doesn't need to be integer. So there is ambiguity how we choose out of the two degenerate particle number non-conserving states the two states with fixed particle number that differs by one. This issue associated with particle number non-conserving approximation also manifest itself in Galilean invariance discussed in Section 3.1.3 where average particle number change due to an extra quasiparticle is not equal to one in the mean-field BCS approximation and in Berry phase calculation in annulus discussed in Section 4.3.3 where again the average particle number with one localized quasiparticle is not increased by one compared to that in the absence of any quasiparticle.

The second issue is on the structure of ground state wave functions. In the last section, we have shown that assuming two degenerate ground states both with even particle number can be both written in BCS paired form, it's not possible to relate them by flipping one pair. Here I want to point out that it is actually impossible for both of them to be written in paired form in the mean-field BdG framework. In fact, paired form for both of them contradicts braiding statistics derived in the BdG framework. As we have seen in discussion in Section 2.6 which applies to a system with four vortices as well that after interchanging two vortices, the monodromy phase (i.e., the phase from instantaneous eigenstate evolution) of two doubly degenerate ground states (which we denote here by $|00\rangle$ and $|11\rangle$ and which we choose to be diagonal with respect to the interchange, i.e., they don't mix into each other) differs by $\pi/2$. On the other hand, if they were both written in paired form, there can be no relative monodromy phase between them. This is due to the fact that under the assumption, each particle number non-conserving state can be written in linear superposition of states each with fixed integer number of Cooper pairs whose number differ from neighboring state in the superposition by one. For a state to evolve back to itself after braiding up to a phase, the monodromy phase of Cooper pair wave function has to be integer number of 2π. Otherwise, states with different number of Cooper pairs would pick up different phases and a particle number non-conserving state, as superposition of them, can't evolve back to itself. So at least for one of the two degenerate ground state, Cooper pair wave function can not be defined in the sense of paired form (it is of course still well defined in the sense of long range order parameter).

The second issue could potentially complicate our treatment of fixing particle number in the following way. To implement constant particle number, there are two obvious approaches. We can either project particle number non-conserving states onto states with fixed particle number by Anderson trick (for odd particle number states, Anderson trick can be aslo applied by including overall superconducting phase factors to Bogoliubov quasiparticle operator: $\alpha^\dagger = \int dr\ \exp\{i\theta/2\}u(r)\psi^\dagger(r)+$

$\exp\{-i\theta/2\}v(r)\psi(r)$ and integrating over $\int d\theta\ \exp\{-i(N+\frac{1}{2})\theta\}$ to get $2N+1$-particle state from a particle number non-conserving state) or we can associate a Cooper pair to the BdG quasiparticle operator to make it particle number conserving. The former way turns out to be too difficult to proceed in practice as states with different superconducting phases (which comes from integrating over superconducting phases by Anderson trick to project from particle number non-conserving states onto states with fixed particle number) have non-vanishing overlaps that complicate calculating Berry phase. So we adapt the latter approach in the following. However, Cooper pair wave function may not be defined in the sense of completely paired form as we just demonstrated above. Keeping this in mind, we now proceed to discussing braiding two vortices.

5.2.1 Two Vortices

As we have seen in Section 2.6, interchanging two vortices resulting in monodromy phase of $\pi/2$ while the Berry phases for two degenerate ground states are the same due to cancellation of particle and hole contributions of Majorana zero modes. Now we want to enforce fixed particle number so that state $|1(\theta_0)\rangle$ has one more particle than $|0(\theta_0)\rangle$. So we associate a Cooper pair to hole part of BdG quasiparticle creation operator and replace expression (2.24) by the following

$$\gamma_i(\theta_0) = \int d^2 r u_i(r,\theta_0)\psi^\dagger(r) + v_i(r,\theta_0)\psi(r)C^\dagger(\theta_0), \tag{5.13}$$

where $C^\dagger(\theta_0)$ adds a Cooper pair to $|0(\theta_0)\rangle$.

Now we investigate braiding statistics in the presence of Cooper pair. As Cooper pair is explicitly taken into account in quasiparticle operator, we need to understand how it evolves under interchange and how it contributes to the Berry phase. As analytic form of Cooper pair wave function is unavailable in the presence of vortices, we have to make some intuitively plausible argument on its structure. Fortunately, the argument can be justified in an equivalent braiding process. We first discuss standard braiding process which we call braiding process I in which vortex 1 and 2 are interchanged as in Section 2.6, followed by an equivalent braiding process which we call braiding process II in which we rotate the whole system by 180°. To take advantage of symmetry and to make use of angular momentum - Berry phase relation found in discussing the annulus model (equation (4.3)), we consider system boundary with perfect rotation symmetry around origin (see figure 2.2)

5.2.1.1 Braiding Process I

The monodromy phase remain the same as given by particle number non-conserving case, i.e., equation (2.30) provided that Cooper pair wave function goes back to itself after interchange which we assume is the case (otherwise, the two ground states don't return to their initial states after interchange).

The Berry phase can be calculated in the same way as in Section 2.6 with equation (2.31). We already knew that the contribution from $u_i(r,\theta_0)$ and $v_i(r,\theta_0)$ vanishes. Now we need to consider the contribution from $C^\dagger(\theta_0)$. We first consider infinite system size where things get simplified. Let's assume that for the Cooper pair wave function, the center of mass and relative coordinates are separable for regions far from the vortices. During the braiding, the Cooper pair dependence on the relative coordinates is unchanged. The center of mass phase of the condensate is also unchanged for regions far away from the two vortices as they can be viewed to be located at origin and hence not moving. So the Cooper pair wave function in the region far from the vortices remains unchanged, i.e., independent of vortex configuration. We could therefore write down the following ansatz for the Cooper pair wave function for regions far from the vortices

$$C^\dagger(\theta_0) = \int dRdr\ \exp(2i\Theta + i\theta)\Psi_c(|R|)\Psi_r(|r|)\psi^\dagger(r_1)\psi^\dagger(r_2), \tag{5.14}$$

where R and r are center of mass and relative coordinates, respectively. Θ and θ are center of mass and relative polar angle, respectively. Ψ_c and Ψ_r denote functions of center of mass and relative coordinates, respectively. They are only functions of magnitude of R and r. The phase factor $\exp(2i\Theta)$ comes from the total vorticity of the vortex pair and the phase factor $\exp(i\theta)$ accounts for internal angular momentum of the Cooper pair of a p+ip superconductor.

Since the dominant part of the Cooper pair comes from regions far from the vortices, it is accurate enough to approximate the Cooper pair wave function by (5.14) and take derivative of it in calculating its contribution to the Berry phase (cf. equation (2.31)). We get vanishing contribution to the Berry phase from the Cooper pair. In the region near the vortices, the Cooper pair wave function is certainly dependent on θ_0, but the point is that the dominant contribution to the Berry phase comes from far regions where the dependence on θ_0 vanishes as the condensate center of mass phase becomes independent of θ_0. So the total braiding phase is the same as given in the particle number non-conserving case, namely $\pi/2$ (see equation 2.32).

We see that the assumption of taking (5.14) to approximate Cooper pair wave function in calculating its contribution to the Berry phase depends on how big the system is compared to the size of region enclosed by interchanging trajectories of the two vortices. If the ratio is of order 1, the approximation is no longer justified. Here we estimate Cooper pair contribution to the Berry phase with a plausible argument. Inside the encircling trajectory, we expect the phase of the Cooper pair wave function to wind by 2π, whereas outside it, there is no phase winding after the encircling. So intuitively, we expect finite contribution from the Cooper pair to the Berry phase. One whole Cooper pair will contribute Berry phase of -2π; since there's only part of the Cooper pair that contributes to the Berry phase, the contribution will be $-2\eta\pi$, where η is the ratio of the area of encircling trajectory to the area of the whole system (see [43] for a related discussion on Cooper pair contribution to Berry phase). One also needs to take into account the fact that the Cooper pair is associated with the hole part of the quasiparticle. So we expect the overall contribution to the Berry phase to be $-\eta\pi$. Of course, this is just an estimate. Rigorous calculation is unavailable at this stage. The point here is that there may well be finite modification to the Berry phase due to the Cooper pair.

5.2.1.2 Braiding Process II

Now let's consider rotating the whole system by 180° about origin. In this case, the Majorana wave functions $u_i(r, \theta_0)$ become

$$\begin{aligned} u_1(r, \theta_0) &= \exp\{(\frac{\pi}{2} - \theta_0)i\}u(|\vec{r} - \vec{R}_1|)e^{i\theta(\vec{r}-\vec{R}_1)} \\ u_2(r, \theta_0) &= \exp\{-\theta_0 i\}u(|\vec{r} - \vec{R}_2|)e^{i\theta(\vec{r}-\vec{R}_2)}. \end{aligned} \tag{5.15}$$

This can be easily derived by first obtaining the solutions to the BdG equations in the rotated frame and expressing the solutions in the original frame as follows. In the rotated frame, the Majorana wave functions are independent of θ_0 since they don't change their configuration in the rotated frame. So their wave functions in the rotated frame are given by their initial ones

$$\begin{aligned} u_1'(r,\theta_0) &= u_1(r,\theta_0=0) = \exp\{\frac{\pi}{2}i\}u(|\vec{r}-\vec{R}_1|)e^{i\theta(\vec{r}-\vec{R}_1)} \\ u_2'(r,\theta_0) &= u_2(r,\theta_0=0) = u(|\vec{r}-\vec{R}_2|)e^{i\theta(\vec{r}-\vec{R}_2)}, \end{aligned} \tag{5.16}$$

where prime superscripts are used to denote solutions in the rotated frame. Since the rotated frame is rotated by θ_0 relative to lab frame, the solutions in the lab frame will pick up phase factor $\exp\{-\theta_0 i\}$, yielding the expression in (5.15). Alternatively, we can compare the BdG equations in the two reference frames. The diagonal terms of BdG equations take the same form, whereas the off-diagonal terms differ by a phase factor $\exp\{-2\theta_0 i\}$ because $\partial_{x'}+i\partial_{y'} = (\partial_x+i\partial_y)\exp\{-\theta_0 i\}$ and the center of mass order parameter in the rotated frame $\triangle' = \triangle\exp\{-\theta_0 i\}$. So when transformed to the lab frame, u_1 and u_2 pick up extra phase factor $\exp\{-\theta_0 i\}$. End of derivation.

After π rotation, the BdG operator $\alpha^\dagger(\theta_0)$ becomes

$$\alpha^\dagger(\pi) = -\alpha^\dagger(0) \tag{5.17}$$

provided that the Cooper pair wave function becomes

$$C^\dagger(\pi) = -C^\dagger(0), \tag{5.18}$$

which will be justified shortly.

Equation (5.17) together with the definition of two degenerate ground states yields the monodromy phase

$$\delta\alpha = \pi. \tag{5.19}$$

Now, let's calculate the Berry phase. Again, the contribution from the derivatives of $u_i(r,\theta_0)$ and $v_i(r,\theta_0)$ vanishes. So we focus on the contribution from the Cooper pair. In this case, both the relative and center of mass coordinates are rotated, so the Cooper pair wave function is dependent on $\theta_i - \theta_0$ for each particle i. Making the similar approximation for regions far from the vortices, we have the same ansatz for the Cooper pair with coordinates replaced by relative ones, i.e., $\theta_i - \theta_0$,

$$C^\dagger(\{\theta_i - \theta_0\}) = \int dRdr\ \exp(2i(\Theta - \theta_0) + i(\theta - \theta_0))\Psi_c(|R|)\Psi_r(|r|)\psi^\dagger(r_1)\psi^\dagger(r_2). \tag{5.20}$$

For infinite systems, by the same approximation made in process I, we use ansatz (5.20) to calculate Cooper pair contribution to the Bery phase. Since $C^\dagger(\{\theta_i - \theta_0\})$ as given by (5.20) is eigenstate of ∂_{θ_0} with eigenvalue $-3i$ and so we get $3\pi/2$ (recall that the Berry phase is calculated by $-\mathrm{Im}\{\int_0^\pi d\theta_0 \langle 0(\theta_0)|\{\alpha(\theta_0), (\partial_{\theta_0}\alpha^\dagger(\theta_0)\}|0(\theta_0)\rangle\}$ and Cooper pair is associated with hole part of Bogoliubov operator which takes half the weight). Together with the π monodromy phase, the total phase is

$$\chi = \delta\alpha + \delta\phi = \pi + 3\pi/2 = 5\pi/2. \tag{5.21}$$

This is equivalent to $\pi/2$ obtained in braiding process I.

The above calculation of Cooper pair contribution to the Berry phase can be understood more intuitively from angular momentum. The Berry phase of the Cooper pair can be regarded as its average angular momentum similar to the situation in the annulus problem. In the thermodynamic limit, the ground state $|0\rangle$ can be regarded as possessing rotation symmetry since both vortices are at the center viewed from large distances. So the Cooper pair wave function can be regarded as eigenstate of angular momentum with eigenvalue 3. As Cooper pair is associated with quasiparticle hole which takes half weight of the quasiparticle, so the contribution to the Berry phase is $3\pi/2$.

For a finite system with rotation symmetry, we can make similar argument as we did in braiding process I and we see that inside the interchange trajectory, the contribution from the center of mass phase of the Cooper pair due to two vortices vanishes. So the Berry phase decreases from $3\pi/2$ by amount which is $\eta\pi$, consistent with the Berry phase correction estimated in braiding process I.

Let's compare the Cooper pair wave function ansatz (5.20) with (5.14). Ansatz (5.20) yields an order parameter center of mass phase which is smaller than the phase by ansatz (5.14) by $2\theta_0$. This agrees with the center of mass phase differences of the gap in the two braiding processes. This confirms that the Cooper pair wave function is independent of θ_0 in far regions in the first braiding process. Notice that the total phase difference of Cooper pair wave function between the two processes is $3\theta_0$, with $2\theta_0$ contributing to the center of mass gap phase and θ_0 contributing to the relative gap phase difference, both of which appear in the BdG equations (so the overall phases of the gap in the BdG equations in the two processes differ by $3\theta_0$).

Furthermore, we see that the apparent two different braiding processes I and II yield the same braiding phase. It's thus tempting to ascribe the difference in the two processes to an overall phase factor. This overall phase factor may be regarded as a gauge choice, i.e., choice of instantaneous ground states and we may conclude that the two processes belong to the same physical process. Let's examine the argument in more details. Let's assume the even particle number ground state $|0\rangle$ in the latter process is the same as that in the former with an extra phase factor of $\exp(-i3\theta_0 N/2)$ (compare equation (5.20) with (5.14)). If at the same time, the corresponding BdG operators in the two processes were the same up to a phase factor, then we can conclude that the two processes are identical. With the definition of Majorana fermion operator (5.13), Majorana wave functions in the two processes (2.28), (5.15) and the assumption that $C^\dagger_{II}(\theta_0) = C^\dagger_I(\theta_0)\exp(-i3\theta_0)$ (Roman subscripts refer to the two processes), we explicitly write down the expressions for the BdG operators in the two processes

$$\begin{aligned}
\alpha^\dagger_I(\theta_0) &= \int d^2r\ \exp\{\frac{\theta_0 i}{2}\}(u(|\vec{r}-\vec{R}_1|)e^{i(\theta(\vec{r}-\vec{R}_1)+\pi/2)} + iu(|\vec{r}-\vec{R}_2|)e^{i\theta(\vec{r}-\vec{R}_2)})\psi^\dagger(r) \\
&+ \exp\{-\frac{\theta_0 i}{2}\}(u(|\vec{r}-\vec{R}_1|)e^{-i(\theta(\vec{r}-\vec{R}_1)+\pi/2)} + iu(|\vec{r}-\vec{R}_2|)e^{-i\theta(\vec{r}-\vec{R}_2)})\psi(r)C^\dagger_I(\theta_0),
\end{aligned}$$

$$\begin{aligned}
\alpha^\dagger_{II}(\theta_0) &= \int d^2r\ \exp\{-\theta_0 i\}(u(|\vec{r}-\vec{R}_1|)e^{i(\theta(\vec{r}-\vec{R}_1)+\pi/2)} + iu(|\vec{r}-\vec{R}_2|)e^{i\theta(\vec{r}-\vec{R}_2)})\psi^\dagger(r) \\
&+ \exp\{-2\theta_0 i\}(u(|\vec{r}-\vec{R}_1|)e^{-i(\theta(\vec{r}-\vec{R}_1)+\pi/2)} + iu(|\vec{r}-\vec{R}_2|)e^{-i\theta(\vec{r}-\vec{R}_2)})\psi(r)C^\dagger_I(\theta_0).
\end{aligned}$$

We see that $\alpha^\dagger_{II}(\theta_0)$ is proportional to $\alpha^\dagger_I(\theta_0)$ by a phase factor $\exp\{-3\theta_0/2i\}$. So we may indeed identify the two processes!

5.2.2 Four Vortices

In the above section, we have compared braiding phases of doubly degenerate ground states whose particle numbers differ by one. We see that in the thermodynamic limit, the result is the same as obtained in particle number non-conserving approximation. However, we notice that finite system size may affect the Berry phase with contribution from Cooper pair. Since we have been comparing states with different particle number parity, the Berry phase we discussed above is Abelian phase. It is much more interesting to consider states with same particle number and possibility of Non-Abelian phase by MZM. For this, we need to consider systems in the presence of at least four vortices. In this case, rigid body rotation considered above in braiding process II is not useful for process of interchanging two vortices while keeping the other two at rest. So we'll have to reply on intuitive argument given in braiding process I above. In the thermodynamic limit, interchanging two vortices has negligible effect on Cooper pair since it is spread over an infinitely large region. So we expect Cooper pair to have vanishing effect on the Berry phase and hence the standard result based on particle number non-conserving approximation is unchanged. For finite systems, the argument is more speculative. As the total number of Cooper pairs (however, we should keep in mind that their definition for both degenerate ground states is subtle) is the same for the two states, we expect the contribution due to Cooper pair to be the same for them. Hence, there's probably no finite size effect.

Our main conclusion is that enforcing fixed particle number while still considering many-body states constructed from BdG equations won't change the conclusion on braiding statistics in particle number non-conserving approximation. However, as we have seen in studying the toy model in Chapter 4 and also in the discussion of many-body wave functions that obey sum rules in Section 3.1.2, the modification of many-body wave functions beyond BdG equations may play an essential role in determining topological properties of MZM in superconductors. We next turn to discussing Majorana physics beyond BdG equations.

5.3 Condensate Deformation and its Effect on Local Particle Number Density

As is explicit in the above consideration of Cooper pair contribution to Berry phase in interchanging two MZM, if the Cooper pair ($C^{\dagger}(\theta_0)$ in the particle number conserving form of BdG quasiparticle given by equation 5.13) in association with the quasiparticle hole is not spread out over all regions but is localized at the quasiparticle, then it may contribute nontrivially to the Berry phase as it undergoes large change when dragged along with the local MZM in the braiding process. To study the possibility of Cooper pair localization due to the presence of localized quasiparticle, we need to go beyond the framework of mean-field BdG equations. Before turning to studying Majorana physics, we would like to get some physical understanding of effect of a localized BdG quasiparticle on many-body wave functions in general. We discuss first how condensate is modified due to the presence of a bound quasiparticle in Section 5.3.1. Then we address the question whether a bound quasiparticle can change local particle number density by a model of Josephson junction taking into account particle number conservation in Section 5.3.2. Finally in Section 5.3.3, we discuss how general considerations of effect of localized quasiparticle beyond particle number non-conserving approach can be related to case with MZM which is special due to its topological nature as predicted by BdG equations.

5.3.1 Condensate Localization due to a Localized Quasiparticle

As we show in Section 3.1.2, the mean-field BCS ground state wave function violates particle number conservation as evidenced by finite long wavelength density fluctuation. To satisfy particle number conservation and prevent long wavelength density fluctuation, we need to modify ground state wave function by taking into account long wavelength collective mode (Anderson-Bogoliubov mode) in a neutral superconductor or collective plasmon mode in a charged superconductor. Intuitively, particle number conservation enforce finite compressibility which disfavors low energy long wavelength density fluctuation. It is natural to wonder whether this effect plays a role in quasiparticle - condensate interaction. We know in the mean-field BdG framework, quasiparticles are independent of each other and condensate is regarded as effective c-number background field. Once particle number conservation is taken into account, the presence of quasiparticles will affect the condensate. Imagining adding a quasiparticle to the condensate, its particle and hole part will change the particle number of the system differently. To conserve particle number, Cooper pair has to be associated to the hole. As one more net particle is added to the system by the quasiparticle, the system state needs to adjust itself to find the new lowest energy configuration. This effect is completely absent in the particle number non-conserving picture as there is no energy cost in changing Cooper pair number.

The above speculation on quasiparticle condensate interaction is supported by a closer examination of BdG equations. To demonstrate this, let's first evaluate BdG quasiparticle energy in the mean-field approach. A quasiparticle energy can be found as

$$E = \langle \alpha H \alpha^\dagger \rangle - \langle H \rangle, \tag{5.22}$$

where $\alpha^\dagger$ denotes quasiparticle creation operator, $\langle\rangle$ refer to taking expectation value in the ground state, H is superconductor Hamiltonian. We can evaluate the above equation by rewriting it as

$$\langle \alpha H \alpha^\dagger \rangle - \langle H \rangle = \langle \{\alpha, [H, \alpha^\dagger]\} \rangle, \tag{5.23}$$

which is valid as long as we require quasiparticle to satisfy $\{\alpha, \alpha^\dagger\} = 1$ and $\alpha|\mathrm{GS}\rangle = 0$. Evaluating equation (C.8) by substituting in the explicit form of the quasiparticle

$$\alpha^\dagger = \int dr u(r)\psi_\uparrow^\dagger(r) + v(r)\psi_\downarrow(r), \tag{5.24}$$

we get the BdG form of quasiparticle energy

$$\begin{aligned} \langle \{\alpha, [H, \alpha^\dagger]\} \rangle &= \int dr u^*(r) H_\uparrow u(r) - V_0 \int dr u^*(r) v(r) \langle \psi_\downarrow(r) \psi_\uparrow(r) \rangle \\ &- \int dr v^*(r) H_\downarrow v(r) - V_0 \int dr u(r) v^*(r) \langle \psi_\uparrow^\dagger(r) \psi_\downarrow^\dagger(r) \rangle, \end{aligned} \tag{5.25}$$

where $H_\uparrow$ and $H_\downarrow$ are single body energy associated with particle and hole respectively. V_0 is

BCS contact potential for s-wave pairing channel. To localize a quasiparticle, we consider here imposing a Zeeman trap similar to what we have considered in annulus model in Chapter 4 but not limited to 1d. The terms in the BdG quasiparticle energy that involve particle particle interaction and superconducting condensate are the off-diagonal terms $-V_0 \int dr u^*(r) v(r) \langle \psi_\downarrow(r)\psi_\uparrow(r)\rangle$ and its complex conjugate (they are called off-diagonal since they mix particle wave function $u(r)$ with hole wave function $v(r)$). We can regard $-V_0 \int dr u^*(r) v(r) \langle \psi_\downarrow(r)\psi_\uparrow(r)\rangle$ as inner product between ground state wave function and wave function created by acting operator $-V_0 \int dr u^*(r) v(r) \psi_\downarrow(r)\psi_\uparrow(r)$ on the ground state wave function. If we restore the Cooper pair associated with the quasiparticle hole, this term becomes $-V_0 \int dr u^*(r) v(r) \langle \psi_\downarrow(r)\psi_\uparrow(r)\Omega^\dagger\rangle$ where $\Omega^\dagger$ refers to a Cooper pair creation operator whose form doesn't have to be the same as those in the superconducting condensate (it is the same in the mean-field approximation). The particle number conserving form of the off-diagonal term can be similarly regarded as inner product between ground state acted on by operator $-V_0 \int dr u^*(r) v(r) \psi_\downarrow(r)\psi_\uparrow(r)$ and ground state added by an extra Cooper pair $\Omega^\dagger$. As we allow extra degree of freedom in $\Omega^\dagger$, we may possibly optimize the off-diagonal term beyond mean-field BdG equations. The hint on how to modify the extra Cooper pair wave function comes from observing the form of $V_0 \int dr u(r) v^*(r) \psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r)|\text{GS}\rangle$. For simplicity, we consider quasiparticle wave function localization size to be much larger than the superconducting coherence length which can be achieved by imposing a wide Zeeman trap with similar size. Writing $\int dr u(r) v^*((r)\psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r)$ in momentum space as $\sum_q f_q \sum_k a^\dagger_{k+q/2,\uparrow} a^\dagger_{-k+q/2,\downarrow}$ with f_q Fourier component of function $f(r) \equiv u(r)v^*(r)$, we expect only wave vectors near Fermi surface have significant contribution to the inner product. Around Fermi surface, $a^\dagger_{k+q/2,\uparrow} a^\dagger_{-k+q/2,\downarrow}$ can be replaced by $a^\dagger_{k+q/2,\uparrow} a_{k-q/2,\uparrow} a^\dagger_{k-q/2,\uparrow} a^\dagger_{-k+q/2,\downarrow}$ in the sense that the two operators are identical when acting on $|\text{GS}\rangle$. The latter operator may be further approximately identified to be spin up density fluctuation operator times a Cooper pair operator, namely, we may identify the product of the first two operators as spin up density fluctuation operator and the product of the latter two as Cooper pair operator. Alternatively, we may approximate $a^\dagger_{k+q/2,\uparrow} a^\dagger_{-k+q/2,\downarrow}$ as spin down density fluctuation operator times a Cooper pair operator. As q is much less than inverse of coherence length, the two approximate expressions can be combined to become a total particle number density fluctuation operator times a Cooper pair operator. So the effect of operator $V_0 \int dr u(r) v^*(r) \psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r)$ on ground state resembles that of a particle number density fluctuation operator, i.e., it creates density fluctuations to the ground state up to momentum $q \sim d^{-1} \ll \xi^{-1}$ (d refers to quasiparticle size, ξ is coherence length). As off-diagonal terms save energy due to attractive superconducting pairing, it is energetically favorable to increase the magnitude of the inner product. Therefore, it is plausible to modify the extra Cooper pair wave function to build in density fluctuations with wave vectors up to $q \sim d^{-1}$. So we write the following ansatz for the modified Cooper pair wave function

$$\Omega^\dagger = \lambda_0 \Omega_0^\dagger + \sum_{q \neq 0, q \leq d^{-1}} \lambda_q \Omega_q^\dagger, \tag{5.26}$$

where $\Omega_0^\dagger$ takes the same form as in the condensate, i.e., $\Omega_0^\dagger = \sum_k C_k a_{k,\uparrow}^\dagger a_{-k,\downarrow}^\dagger$ and $\Omega_q^\dagger$ creates condensate Cooper pair boosted by momentum q, i.e., $\Omega_q^\dagger = \sum_k C_k a_{k+q/2,\uparrow}^\dagger a_{-k+q/2,\downarrow}^\dagger$.

Now the crucial question is whether the modification of $\Omega^\dagger$ due to the localized quasiparticle is finite in the thermodynamic limit. Let's first attempt to quantify the degree of modification by comparing the relative weight of many-body wave functions created by acting $\lambda_0 \Omega_0^\dagger$ and by acting $\sum_{q \neq 0, q \leq d^{-1}} \lambda_q \Omega_q^\dagger$ on the ground state. Let's require the normalization condition for $\Omega_0^\dagger$ be such that $\langle \Omega_0 \Omega_0^\dagger \rangle = 1$ where expectation value is taken in the BCS ground state. By requiring the modified Cooper pair to be normalized as well, i.e., $\langle \Omega \Omega^\dagger \rangle = 1$, we get the following constraint on λ_0 and λ_q

$$|\lambda_0|^2 + \sum_q |\lambda_q|^2 \frac{\triangle}{N \epsilon_F} = 1, \tag{5.27}$$

where N is total particle number, $\triangle$ and ϵ_F are superconducting gap and Fermi energy respectively. The first and second term in the above equation represents normalization from $\lambda_0 \Omega_0^\dagger$ and $\sum_q \lambda_q \Omega_q^\dagger$ respectively. As the number of different q is of order $N(\triangle/\epsilon_F)^3$ in 3d, we see that the normalization of $\sum_q \lambda_q \Omega_q^\dagger$ is of order $(\triangle/\epsilon_F)^4$ compared to that of $\lambda_0 \Omega_0^\dagger$ if we assume each $|\lambda_q|$ is on the same order of magnitude as $|\lambda_0|$. (The justification for estimating number of different q: The magnitude of q is bounded by d^{-1} which is smaller than ξ^{-1}. If we take ξ^{-1} as our upper bound, the maximum magnitude of q is $(\triangle/\epsilon_F) q_F$. Integrating over different q, the total number of q is of order$N(\triangle/\epsilon_F)^3$. The actual number of q is smaller by another factor of $(\xi/d)^3$, which we didn't include only for notation simplicity. But the qualitative result is unaffected since we are interested in knowing whether the modification of many-body wave function due to bound quasiparticle is independent of system size.) So the modification can be finite in the thermodynamic limit. In evaluating the normalization in equation 5.27, we have used BCS ground state. If we include long wavelength collective mode in case of neutral superconductor, we may estimate normalization of $\Omega_q^\dagger|\mathrm{GS}\rangle_{\mathrm{coll}}$ ($|\mathrm{GS}\rangle_{\mathrm{coll}}$ refers to ground state wave function taking into account long wave length collective Anderson-Bogoliubov modes) by replacing $\Omega_q^\dagger$ with density fluctuation operator ρ_q. Then the normalization of $\Omega_q^\dagger|\mathrm{GS}\rangle_{\mathrm{coll}}$ becomes normalization of $\rho_q|\mathrm{GS}\rangle_{\mathrm{coll}}$, namely, the long wave length density fluctuation in the ground state, which is

$$\langle \rho_q \rho_{-q} \rangle = \frac{nq}{mc} \sim q\xi \frac{\triangle}{\epsilon_F} \frac{n}{V}, \tag{5.28}$$

where in evaluating density fluctuation, we have used hydrodynamic description for the effective Hamiltonian, n is particle number density and V is system volume. So its relative weight to that of $\Omega_0^\dagger|\mathrm{GS}\rangle_{\mathrm{coll}}$ which is similarly estimated to be $\langle \rho_0^2 \rangle = n^2$ is $q\xi \triangle /(N\epsilon_F)$. This estimation is similar to evaluation based on BCS ground state and is smaller by a factor of $q\xi$ as result of vanishing long wavelength density fluctuation. As we evaluate relative weight of wave functions by integrating $q\xi$ over all $q \leq d^{-1}$, we get the same order of magnitude estimate as above, i.e., $(\triangle/\epsilon_F)^4$ multiplied by a numerical factor much smaller than 1. But the qualitative conclusion is the same, i.e., the modification of many-body wave functions due to modified extra Cooper pair is finite in the thermodynamic limit if ratio of $|\lambda_q|/|\lambda_0|$ for each q is finite in the thermodynamic limit.

As we have shown it is plausible to expect finite modification of many-body states by modifying the extra Cooper pair added to the ground state, we now need to actually show that $|\lambda_q|/|\lambda_0|$ is finite in the thermodynamic limit and it will be ideal to further find analytic form for λ_q. Although it's tempting to minimize quasiparticle energy given by equation 5.25 with Cooper pair operator added to the off-diagonal terms, it turns out to be very difficult (see appendix C). Once we consider a localized Cooper pair, the standard BdG energy needs to be modified by including contribution from it and the resulting form is complicated. Even more difficult issue comes from normalization. Once we explicitly take into account Cooper pair, we need to enforce particle number conservation explicitly. We need to enforce both the particle number after adding a localized quasiparticle and the corresponding normalization which turn out to be very messy to implement. Furthermore, it is also unclear whether we need to take into account collective modes for the ground state to be consistent with the modified Cooper pair. Therefore, we present in the following qualitative estimate on the degree of modification of the added Cooper pair.

Before analyzing Cooper pair modification, it's instructive to recall quantum mechanics of single particle in potential well. We know that a particle is either completely localized inside the well or completely delocalized as plane waves. The condition of localization depends on strength of potential well as well as dimension. In 1d, a particle is always localized no matter how weak the potential trap is. In higher dimensions, localization depends on strength of potential well. If the extra Cooper pair could be effectively regarded as single particle in effective potential trap due to the presence of localized quasiparticle, then we expect it is either completely localized or completely delocalized. In the former case, the extra Cooper pair would be completely localized at the location of quasiparticle. Whereas in the later case, the modification to Cooer pair due to local quasiparticle is vanishing in the thermodynamic limit. On the other hand, the problem of finding the extra Cooper pair state is inherently a many-body problem and it may not be simplified to a single particle Schrodinger problem. We shall now show that indeed the localization of the extra Cooper pair is different from single particle quantum mechanics.

For qualitative argument, we shall satisfy ourselves with particle number non-conserving version of modified BdG quasiparticle wave function. We consider two trial wave functions (with odd particle number due to one localized quasiparticle which can is localized by a weak Zeeman field): the standard many-body wave functions according to the mean-field BdG description and the many-body wave function with modified quasiparticle states and examine whether there's finite mixing between them for a variational ground state as linear superposition of them. The BdG many-body wave function with a localized quasiparticle is

$$\Psi_0 = \sum_q \beta_q a^\dagger_{q\uparrow} \prod_{k\neq q} (u_k + v_k b^\dagger_k)|\mathrm{vac}\rangle, \tag{5.29}$$

where q is around the Fermi surface satisfying $\epsilon_q \ll \triangle$, $b^\dagger_k \equiv a^\dagger_{k,\uparrow} a^\dagger_{-k,\downarrow}$. The many-body wave function containing one modified Cooper pair is

$$\Psi_1 = \sum_q \beta_q a^\dagger_{q\uparrow} \sum_{q'\neq 0} \lambda_{q'} \sum_{k'\neq q\pm q'/2} C_{k'} b^\dagger_{k',q'} \prod_{k\neq q,k'\pm q'/2} (u_k + v_k b^\dagger_k)|\mathrm{vac}\rangle, \tag{5.30}$$

where q' has magnitude no bigger than $d^{-1} \ll \xi^{-1}$ and $b^\dagger_{k',q'} = a^\dagger_{k'+q'/2,\uparrow} a^\dagger_{-k'+q'/2,\downarrow}$. By construction, Ψ_1 is orthogonal to Ψ_0. To satisfy normalization condition of Ψ_0 and Ψ_1, β_q is of order $1/\sqrt{N_q}$, $\lambda_{q'}$ is of order $1/\sqrt{N_{q'}}$ and $C_{k'}$ is of order $1/\sqrt{N}$, where N_q, $N_{q'}$ are number of different q and q' that are summed over, respectively and N is total average particle number.

A few remarks on the choice of two wave functions (5.29) and (5.30) are needed before we proceed. They are not exactly the two trial states we mentioned. For simplicity and clarity, I have orthogonalized the two trial states. Furthermore, strictly speaking, the coefficients of operator $a^\dagger_{q\uparrow}$ for the two orthogonalized states (5.29) and (5.30) are not the same as they are from particle and hole wave function $u(r)$ and $v(r)$ (cf. equation 5.24) respectively. However, they are close to each other for a bound quasiparticle state. Hence for the sake of simplicity, we approximate them to be the same without affecting the qualitative conclusion.

Now let's consider the matrix element $\langle\Psi_0|H|\Psi_1\rangle$ with H given by

$$H = \sum_{k,\sigma} \epsilon_k a^\dagger_{k\sigma} a_{k\sigma} - V_0 \sum_{k,k',q} b^\dagger_{k',q} b_{k,q}, \tag{5.31}$$

where I have omitted the Zeeman term for simplicity. Straightforward calculation yields the following estimate

$$\begin{aligned}
\langle\Psi_0|H|\Psi_1\rangle &= V_0 \sum_{q,q',k'} \beta_q \beta_{q+q'} \lambda_{q'} C_{k'} (v_q u_{k'+q'/2} u_{k'-q'/2} - u_q v_{k'+q'/2} u_{k'-q'/2}) \\
&\sim V_0 \frac{1}{N_q} \frac{1}{\sqrt{N_{q'}}} \frac{1}{\sqrt{N}} N_q N_{q'} N \frac{\triangle}{\epsilon_F} \\
&\sim V_0 \sqrt{N N_{q'}} \frac{\triangle}{\epsilon_F} \\
&\sim \triangle \sqrt{N_{q'}/N}.
\end{aligned} \tag{5.32}$$

We see that the matrix element is independent of system size. In fact, we can make it even bigger by constraining $C_{k'}$ in (5.30) in a thin shell around the Fermi surface, since only single particle sates near the Fermi surface can be scattered by the BCS potential. The coupling between Ψ_0 and Ψ_1 is due to scattering of pairs of particles in Ψ_0 by non-zero center of mass momentum scattering terms $-V_0 \sum_{k,k',q\neq 0} b^{\dagger}_{k',q} b_{k,q}$.

We expect that the diagonal energy difference between $\langle \Psi_0 | H | \Psi_0 \rangle$ and $\langle \Psi_1 | H | \Psi_1 \rangle$ to be independent of system size since Ψ_1 is different from Ψ_0 only by a localized Cooper pair. Since both this energy difference and the off-diagnoal energy $\langle \Psi_0 | H | \Psi_1 \rangle$ are independent of system size, the variational ground state is superposition of the two states Ψ_0 and Ψ_1 whose weights are independent of system size. Hence we reach the conclusion that modification of extra Cooper pair due to localized quasiparticle is finite in the thermodynamic limit. In the sense of Cooper pair localization, we may say the extra Cooper pair is partially localized since weights of many-body states corresponding to unmodified extra Cooper pair (and therefore unlocalized) and to modified Cooper pair (completely localized with the size of that of the bound quasiparticle) have the same order of magnitude in the ground state with odd number of particles. This is indeed different from bound state of single particle quantum mechanics.

Intuitively, the partially bound Cooper pair may be understood as follows. Imagine we start with the mean-field many-body eigenstate with one localized quasiparticle and consider its evolution in time. When a Cooper pair is near the region of localization, it gets deformed due to Cooper pair quasiparticle interaction. The percentage of time spent by a Cooper pair near the localization region is vanishing in the thermodynamic limit. However, all Cooper pairs get the same modification, so the effect from all Cooper pairs adds up to compensate the small deformation of each Cooper pair. From this perspective, the more physical ansatz beyond BdG construction for superconducting many-body eigenstates in the presence of localized quasiparticle should modify all Cooper pairs in the condensate, not just one pair associated with the quasiparticle hole.

We have shown that in general, superconducting condensate can have finite local deformation due to a localized quasiparticle. The next interesting question to ask is whether such deformation has any physically observable effect. We shall focus on the simplest observable, the particle number density. This is the subject of the next section.

5.3.2 Particle Localization by a Bound Quasiparticle - a Zeeman-Josephson Model

Knowing that the condensate is deformed doesn't directly tell us what happens to particle number density. In fact, it's impractical to calculate particle number density explicitly even if we know the many-body eigenstate in the presence of a localized quasiparticle which would take complicated form. Furthermore, even if we can evaluate it numerically, it wouldn't tell us much about the underlying physics. So we shall look for physics related to conserved particle number which is the key physics missing in the particle number non-conserving BdG physics.

One type of such simple models suitable for our consideration is superconducting charge qubits made of Josephson junctions. We consider a system made of two superconducting grains joined by a Josephson junction. The total particle number of the system is conserved. The effective Hamiltonian can be written as

$$H = E_C(n - n_g)^2 - E_J\cos\phi. \tag{5.33}$$

The first term corresponds to charging energy which depends on particle number change n between two superconducting grains due to Cooper pair transfer between two sides (we have rescaled E_C to make n particle number change between two superconducting grains, note that in the original definition, n refers to Cooper pair transfer between two superconducting grains, see more detailed explanation below). The second term is responsible for Josephson tunneling energy, ϕ is relative phase difference between the two superconducting grains. n_g is offset induced by gate voltage in the original transmon model and it doesn't need to take integer values. This simple Hamiltonian has been solved exactly.

For our purpose, we would like to apply the above Hamiltonian to describing the same system, but with total odd number of particles and a uniform weak Zeeman field acting on the left grain (see figure 5.1). In other words, we want to study the quasiparticle localized by a Zeeman field in the context of a Josephson junction. The effective Hamiltonian 5.33 is a minimal Hamiltonian describing competition between energy which tends to fix particle number and energy which favors particle number fluctuation in each grain. We believe it is the right model to capture the essential physics of particle number localization for our case.

To adapt Hamiltonian 5.33 to our Zeeman-Josephson system, we need to make some assumptions. We need to assume the unpaired particle contributes to the charging energy (the first term) equally as that of each paired particle and it doesn't change E_C. We further assume the Zeeman field is such that the unpaired particle is only residing on the left side, namely, we ignore single particle tunneling process across Josephson junction. Under these assumptions, the left side grain is in mixture of odd number of particles whereas the right side even number of particles. In the absence of the unpaired particle (when the system has even number of particles), we set $n_g = 0$. In the presence of the unpaired particle, we assume its effect is to change n_g to 1 for the following reason. We have rescaled E_C such that n refers to particle number change between two sides. For example, two particle transferring from left to right is equivalent to four particle change $n = 4$. In infinite E_J limit, we expect no extra particle localized on the left grain due to the localized quasiparticle , but only a net spin localized on the left. In other words, in the infinite E_J limit, the average particle number is increased by one half on both sides due to one added particle in the ground state. So the expectation value of n in the ground state should equal to 1 ($\langle n \rangle = 1$), namely on average, a quarter of Cooper pair (that is half a particle) is transferred from left to right to compensate one more particle added to the left. Therefore $n_g = 1$ according to Hamiltonian 5.33 since in the infinite E_J limit, $\langle n \rangle = n_g$.

Since we have justified using an effective Hamiltonian 5.33 with $n_g = 1$ to calculate the ground state of our Zeeman-Josephson system with odd number of particles, we can make use of available analytic result to evaluate average particle number change $\langle n \rangle$ for finite but large E_J/E_C. By

Feynman-Hellman theorem, $\langle n \rangle$ in the ground state can be related to ground state energy derivative

$$\begin{aligned}
\langle n \rangle &= \frac{1}{2E_c}\langle\frac{\partial H}{\partial n}\rangle + n_g \\
&= -\frac{1}{2E_c}\langle\frac{\partial H}{\partial n_g}\rangle + n_g \\
&= -\frac{1}{2E_c}\frac{\partial E_0}{\partial n_g} + n_g,
\end{aligned} \tag{5.34}$$

where E_0 is ground state energy.

We can now apply analytical solutions found by Koch et al. [44] to evaluate 5.34. Noticing the difference between energy scale E_C, the derivative $\partial E_0/\partial n_g$ is actually taken at $n_g = 1/4$ in their definition. We get the following estimate for $\langle n \rangle$

$$\langle n \rangle = 1 - f(E_J/E_C)\text{exp}(-\sqrt{2E_J/E_C}), \tag{5.35}$$

where $f(E_J/E_C) > 0$ is a power law function of E_J/E_C whose specific form is not very important here due to the exponential factor.

We see from 5.35 that the particle number transfer due to Cooper pairs from left to right is smaller than one half by amount which is exponentially small! The point of our interest is that when finite charging energy E_C is taken into account, there is net particle localization on the left due to the localized quasiparticle. So we have shown that particle number conservation can lead to net particle localization.

It is still nontrivial to generalize argument in the above model to actual situations with a localized quasiparticle. But intuitively, we can think of the region of localized quasiparticle as one superconducting grain and the rest as the other grain. Finite compressibility induces charging energy cost in particle number fluctuation in each region whereas Josephson energy favors particle number fluctuation. In the thermodynamic limit, the ratio of Josephson energy to charging energy stays finite and hence we expect finite particle localization. Of course, there are very important differences between a localized quasiparticle in superconductor and Zeeman-Josephson model. In actual situations of interest, there's no real Josephson junction separating the two regions and no constraints on particle number parity in either region. It is much more difficult to evaluate the effect of particle localization in more physically relevant systems and we leave it to future study.

5.3.3 Local Distinguishability of Localized Majorana Zero Modes?

We have gathered through the above two sections rather convincing evidence for finite superconducting condensate deformation in the thermodynamic limit due to a localized quasiparticle and the resulting local particle number density change. Now the big question is whether conclusions drawn in general also hold in the case of Majorana zero modes. If it turns out to be the case, then we'll have to re-examine the whole basis of topological quantum computing based on MZM in superconductors. This is not just because the braiding statistics of MZM may be modified, but more seriously, the very nature of topological protection exhibited by MZM may be spoiled due to local particle number density modification induced by MZM. If locally we can distinguish degenerate ground states related by MZM, it is even questionable whether one physical degree of freedom associated with a zero energy quasiparticle is split at two spatially separate locations where MZM reside. The very existence of MZM could be questionable and we may possibly end up having only ordinary localized zero energy quasiparticles. So it is of great interest to address the question.

Topologically speaking, the physics of MZM is very different from ordinary localized quasiparticles according to mean-field BdG formalism. For a general local quasiparticle, the local superconducting order parameter is modified due to its presence. This can be easily seen by expanding $\psi(r)\psi(r')$ in BdG quasiparticles when evaluating the order parameter and the presence of a local quasiparticle change the occupation number of the corresponding BdG quasiparticle. Since it is local, its wave function has finite weight locally and contributes a finite amount to local order parameter in the thermodynamic limit. In this sense, the conclusions we reached in the above two sections come as no surprise. On the other hand, as we've pointed out in Chapter 2, due to non-locality nature of pairs of MZM, no local physical quantities (that preserve particle number parity) are distinct in degenerate ground states related by MZM. We can easily confirm this for the superconducting order parameter by an explicit calculation as outlined for the case of a general local quasiparticle. So any modification (for instance, taking into account Hartree-Fock terms self-consistently in deriving BdG equations as is done in nuclear physics) starting from the BdG framework is not going to yield qualitative new physics of MZM. Therefore it is very difficult to go beyond mean-field BdG framework for new physics in MZM. At present, we don't know how to generalize considerations in the above two sections to studying potential new physics in MZM. Below, I shall give a very speculative argument supporting the possibility of new physics in MZM beyond mean-field BdG approximations.

In order to show that local MZM can modify local superconducting condensate, it's desirable to show some local differences in structures of degenerate ground states related by MZM. To this end, we consider adiabatically evolving two degenerate ground states in the presence of four spatially separate MZM residing in four vortices in a spinless p+ip superconductor. Suppose the two degenerate ground states are related to each other by two zero energy Dirac quasiparticles $\alpha_{12}^\dagger = \gamma_1 + i\gamma_2$ and $\alpha_{34}^\dagger = \gamma_3 + i\gamma_4$, where γ_i, $i = 1, \cdots, 4$ are four Majorana zero modes at four vortices. As we merge vortex 1 with 2 and 3 with 4, the two zero energy modes become finite energy modes. At the same time, the two degenerate states are split in energy. One of them evolves into unique ground state and the other becomes the first excited energy eigenstate. If we are considering even number of particles, we may expect that the unique ground state is completely paired (at BCS mean-field level) and the first excited state has two unpaired particles. Since they are adiabatically evolved from the degenerate ground states, we may expect traces of local structure difference in the two degenerate ground state wave functions at locations of four vortices, for in stance local unpaired particles in one of them. Similarly, for states with odd number of particles, we expect the two ground states to evolve into two ground states with odd number of particles. In the BCS mean-field description, each of the two states has a local quasiparticle sitting in a different merged vortex. Intuitively, we may expect to find a local unpaired particle in each of them that is localized at different vortices. So for the initial degenerate ground states, we may expect unpaired particle in vortex 1 and 2, and vortex 3 and 4 respectively. If this conjecture were true, we may expect local quasiparticle to modify the superconducting condensate, resulting in differences between degenerate ground states beyond mean field description. So I conclude that it is rather possible that there is indeed new physics concerning MZM beyond predicted by BdG equations, which fulfills the main purpose of this thesis to raise attention in the physics community to reexamine Majorana physics in superconductors and the whole business of using Majorana zero modes for topological quantum computing.

5.4 Figure

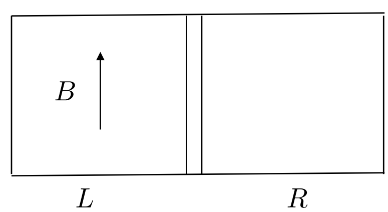

Figure 5.1: Josephson-Zeeman model. We consider two superconducting grains L and R connected by a insulating junction. The total number of particles is odd. A quasiparticle with spin up is localized in the left superconducting grain due to a uniform Zeeman field imposed on the left grain.

Chapter 6

Summary and Outlook

In this thesis, we have examined the validity of mean-field theory and BdG equations for studying topological properties of Majorana zero modes in superconductors. The mean-field BCS and BdG framework describes many-body quantum states which are coherent superposition of different particle numbers. They are constructed for mathematical convenience (and are somewhat 'misleadingly' called $U(1)$ symmetry-breaking), but are not physical states. This is of special concern in the context of quantum information and quantum computing where quantum coherence is of most importance. It is thus natural to question whether physical states with fixed particle number exhibit same quantum properties useful for topological quantum computing. Furthermore, all topological properties concerning Majorana zero modes are derived in the non-interacting particle picture. In the meanwhile, particle particle interaction is essential for inducing superconductivity in the first place. One may wonder whether non-interacting approximation is adequate.

In fact, the issue of particle number conservation had been extensively discussed in the context of gauge invariance of BCS theory. Collective modes of superconducting condensate need to be included to ensure a gauge invariant theory. Although in most practical situations (for example, for most conventional superconductors) condensate doesn't appear explicitly except for providing off-diagonal long range order, it becomes important when it carries interesting structure and non-trivial dynamics. A famous example is superfluid Helium-3 in which Cooper pairs form triplet pairing with rich spin and orbital structure. In calculating its NMR response, it's the collective response of the condensate that underlies the physics.

As Cooper pair has nontrivial structure manifested by its non-zero internal angular momentum in chiral superconductors that are believed to host Majorana zero modes, it is worth examining its possible effect on Majorana zero modes. The most obvious way to include Cooper pair is to consider particle number conserving form of BdG quasiparticles corresponding to Majorana zero modes. We show explicitly that Cooper pair contributes to the Berry phase when we interchange two vortices in a two-vortex superconductor through its angular momentum, both internal and that induced by vortices. For a finite system, the effect of the Cooper pair to the Berry phase may not be neglected. As for a four-vortex system with four Majorana zero modes to realize doubly degenerate ground states with same particle number, the definition of Cooper pair for both states is problematic as it's impossible for them to both be written in BCS paired form in the mean-field description. Therefore, it is still an open question concerning the effect to the Berry phase and braiding statistics of particle pairs included for particle number conserving form of BdG quasiparticles which connect two degenerate ground states, since the added particle pair creation and annihilation operators can't take the same form in order to for them to connect states with different particle numbers that appear in linear superposition for the particle number non-conserving states. In the thermodynamic limit, we intuitively expect the effect on the Berry phase and braiding statistics of extra Cooper pairs that appear in particle number conserving form of BdG quasiparticles to vanish. However, in any realistic system, as long as a braiding operation covers significant region of the whole system, we may not neglect effect of extra Cooper pair. Calculation in a Kitaev wire network (Appendix A) shows that states with particle number that are different from average particle number yield different braiding statistics than the standard one. As properties of MZM in the mean field approach is completely insensitive to average particle number, it is worth further studying whether corresponding particle number conserving states always share the same braiding statistics by tuning the average particle number in the mean-field approach.

It may not be sufficient to study Majorana properties for particle number conserving states at the mean-field level, i.e., states obtained by projecting particle number non-conserving states in mean-field theory to fixed particle number sectors. Particle number conservation puts more constraints than just writing down states with fixed particle number. They are associated with conservation laws that give various sum rules. As a simple example, for a BCS ground state to satisfy f-sum rule and compressibility sum rule, we need to build in it collective modes of the condensate. Furthermore, we show a toy model that suggests the necessity of condensate deformation in response to a localized quasiparticle in order to satisfy continuity condition and f-sum rule in evaluating Berry phase of transporting the quasiparticle. So particle number conservation suggests that it may not be justified to ignore the many-body effect in studying Majorana physics. We are particularly interested in knowing whether Cooper pairs get deformed by local Majorana zero modes and as a result, whether we can locally distinguish degenerate ground states related by Majorana zero modes. We have attempted to answer these questions for a localized quasiparticle trapped by a Zeeman field. We argued that Cooper pairs are indeed deformed and there is net particle localization as the result of quasiparticle localization in a Zeeman-Josephson model. Both effects survive the thermodynamic limit. The generalization to Majorana zero mode is non-trivial due to its topological nature. Any modification and perturbation starting from the mean-field theory are unlikely to yield qualitatively new physics since topological degenerate ground states are locally indistinguishable. Nevertheless, by examining evolution of degenerate ground states, we may still imagine possible local distinction between them as they can be evolved from states that are locally different. We expect condensate - quasiparticle interaction to modify local wave functions. We leave this to future work.

If local deformation of degenerate ground states by Majorana zero modes is important, this may change braiding statistics and more seriously even destroy local topological protection. Then as many-body effect is important, non-interacting single particle approximation and particle-hole symmetry of BdG solutions can no longer be relied on. Consequently, we can not even be sure of long range quantum entanglement exhibited by a pair of Majorana zero modes. In other words, does Majorana zero modes really exist or we may end up with ordinary zero energy Dirac modes that are not split spatially? In this respect, it is very important to better understand physics of Majorana teleportation which is directly related to long range entanglement of Majorana zero modes and to design relevant experiments for testing it. In the present author's opinion, theoretical work that gives satisfying illustration of non-local property of pairs of Majorana zero modes is lacking. For some of the relevant work, see [45]- [50].

It may also help to explore analogy with other condensed matter systems where Majorana zero modes are predicted to exist. Of particular interest are Moore-Read Pfaffian state at $\nu = 5/2$

filling [51] and Kitaev honeycomb model [52]. In the former state, composite fermions form p+ip pairing at the mean-field level [53]. As for the latter state, it has a mean-field description that is equivalent of p+ip pairing at the particle number non-conserving mean-field level [54] and its exact solution can also be mapped onto mean-field p+ip ground state after non-local Jordan-Wigner transformation [55]. In both cases, mapping between them and p+ip superconductor is not exact as the analogy is only at the mean-field level. Furthermore, in more interesting cases with Majorana zero modes, the mapping between them is still lacking. So we can't conclude yet from properties of Majorana zero modes in those systems that p+ip superconductor has the same property. It may worth further investigating analogy with them, given the more thorough theoretic studies in them, both analytically (e.g., [56]) and numerically (e.g., [57]- [61]).

The Majorana physics in chiral superconductors and its application to topological quantum computing is by no means well understood. While people are putting a lot of effort in looking for Majorana zero modes and designing protocols of using them for quantum computing, I believe it is of equal importance to examine the fundamental basis of Majorana in superconductors more deeply.

Appendix A

Braiding Majorana fermions using 1D Kitaev Network with Conserved Particle Number

In this appendix, we lay out details of calculations of Braiding statistics of Majorana zero mode in 1d Kitaev wire networks with conserved particle number. As mentioned in the main text (Section 3.1.1.1), original Kitaev wire doesn't conserve particle number and we want to consider effective quasi-1d system (3d in physical dimension to support superconducting long range order) with fixed particle number (i.e., it doesn't exchange particles with environment) and use Kitaev wire Hamiltonian (i.e., mean-field BCS Hamiltonian) to first calculate particle number non-conserving many-body eigenstates and then project onto fixed particle number sector to obtain particle number conserving states at the mean-field level. The motivation for doing this is to check wether states with fixed particle number evolve under interchanging MZM in the same way as particle number non-conserving states do. The monondromy phase will not be affected by fixing particle number since states with fixed particle number are obtained by projecting particle number non-conserving states. However, the Berry phase may differ for the two cases as the Berry phase for a particle number non-conserving state is average of Berry phases of states each with fixed particle number. The average is not necessarily equal to its constituents unless there is an equal contribution from every state with fixed particle number.

In order to move Majorana zero modes, we impose some external potentials on the wires so that both chemical potential and particle-particle interactions can be tuned. To keep the calculation physical, there are two criteria to meet during the move.

1. Self-consistent condition or gap equation needs to be satisfied. This requirement may complicate calculations if we had to iterate mean field calculations to achieve self-consistency. Furthermore, we require physically reasonable particle-particle interactions (in our calculations, short

range interaction).

2. Average particle number calculated by the mean field approach needs to be fixed during the braiding. Since we are considering particle number conserving wave functions, the average particle number needs to remain constant before projection.

There is an issue related to the second criterion also discussed in the main text. The second criterion is to ensure particle number conserving wave functions be well approximated by the particle number non-conserving wave functions. In large systems with macroscopic particle number, it may be loosened to allow certain amount of variation in average particle number. It is unclear to what extent this can be done without affecting the braiding statistics.

Furthermore, there's another issue of orthogonality. As particle number conserving wave functions are obtained by projection from particle number non-conserving wave functions which form an orthonormal basis, after projection the wave functions may be slightly non-orthogonal. To calculate braiding statistics self-consistently, we need to use orthonormal basis. As system size becomes large, the degree of non-orthogonality should become small. However, it is not totally clear whether the non-orthogonality decreases fast enough to ensure consistency.

With these caveats, let's proceed to examine braiding in particle number conserved systems. We'll first check in A.1 whether the two criteria can be realized in a simple system. Before embarking on braiding Majorana fermions, we'll briefly review in A.2non-Abelian braiding with an emphasis on gauge invariance which will be useful for simplifying calculation in exchanging two Majorana zero modes. Finally, in A.3 and A.4, we discuss double and single interchange braiding scheme respectively.

A.1 Criteria Check

Fortunately, the two criteria can be satisfied in a relatively straightforward way. Consider a single wire with two open ends described by the following mean-field particle number non-conserving Hamiltonian (i.e., Kitaev wire Hamiltonian)

$$H = \sum_{i=1}^{N-1} (a_i^\dagger + a_i)(a_{i+1}^\dagger - a_{i+1}). \tag{A.1}$$

Defining Majorana fermions as

$$\begin{aligned} \gamma_A &= \frac{a^\dagger - a}{i} \\ \gamma_B &= a^\dagger + a, \end{aligned} \tag{A.2}$$

(A.1) can be written as

$$H = \sum_{i=1}^{N-1} i\gamma_{i,B}\gamma_{i+1,A}. \tag{A.3}$$

There are two zero Majorana modes at the ends $\gamma_{1,A}$ and $\gamma_{N,B}$. It can be easily checked that the order parameter in the ground state is

$$\langle a_{i+1}a_i \rangle = -1/4, \tag{A.4}$$

for any $N > 2$. To satisfy the gap equation, we only need to require the nearest neighbor interaction to be

$$V_{i,i+1} = -4. \tag{A.5}$$

So a physically realistic nearest neighbor interaction suffices to satisfy the self-consistency condition. The full particle number conserving Hamiltonian corresponding to the mean-field approximation

(A.1) is given by

$$H_{full} = \sum_{i=1}^{N-1} -a_i^\dagger a_{i+1} + h.c. - 4a_i^\dagger a_{i+1}^\dagger a_{i+1} a_i. \tag{A.6}$$

Next, let's try to move the left Majorana zero mode γ_{1A} to the right by one site and in the meanwhile move the right Majorana zero mode γ_{2B} to the right by one site in order to keep average particle number constant (see figure A.1). Let the tuning mean-field Hamiltonian to be

$$\begin{aligned} H' &= 2\lambda\mu_1(\lambda)a_1^\dagger a_1 + (1-\lambda)(a_1^\dagger + a_1)(a_2^\dagger - a_2) \\ &+ 2(1-\lambda)\mu_{N+1}(\lambda)a_{N+1}^\dagger a_{N+1} + \lambda(a_N^\dagger + a_N)(a_{N+1}^\dagger - a_{N+1}). \end{aligned} \tag{A.7}$$

(Note that the system Hamiltonian can be read off from the graphic representation such as that shown in figure A.1 (it represents $H + H'$ with H and H' given by equation A.1 or equivalently equation A.3 and equation A.7, respectively) according to the following rules. Each site is represented by two dots corresponding to the real and imaginary part of the fermion on the site. The left dot represents $\gamma_{i,A}$ and the right represents $\gamma_{i,B}$ and the fermion creation operator one the site i is $a_i^\dagger = 1/2(\gamma_{i,A} + i\gamma_{i,B})$. Depending on direction, each link with arrow represents either $i\gamma_{i,B}\gamma_{i+1,A}$ (pointing from site i to site $i+1$) or $i\gamma_{i+1,A}\gamma_{i,B}$ (pointing from $i+1$ to i). A link with varying strength parameterized by λ is represented by a dashed line. Isolated dots represent unoccupied site with positive chemical potential on it.) We require that as λ goes from 0 to 1, both Majorana zero modes are moved to the right by one site. This is easily achieved as long as $\mu_1(\lambda) > 0$ and $\mu_{N+1}(\lambda) > 0$. As shown in figure A.1, at stage (a), there is one Majorana zero mode $\gamma_{1,A}$ sitting at site 1, and one Majorana zero mode $\gamma_{N,B}$ sitting at site N. Site $N+1$ is initially unoccupied. At intermediate stage (b), the strength of the link (i.e., the magnitude of coefficient of $\gamma_{1,B}\gamma_{2,A}$ of the Hamiltonian) between site 1 and 2 decreases whereas the strength of the link between N and $N+1$ increases (remember that the changing strength of links is represented by dashed lines), meanwhile the chemical potential on site 1 increases and that on site $N+1$ decreases. At final stage (c), site 1 is unoccupied and the link between site 1 and 2 vanishes, whereas strength of link between site N and $N+1$ reaches final value. The Majorana zero modes are now sitting at site 2 and $N+1$, respectively. Constant average particle number during the process can be achieved by tuning functions $\mu_1(\lambda)$ and $\mu_{N+1}(\lambda)$. Explicit calculation shows that the order parameters $\langle a_{i+1}a_i\rangle$ for $i = 2, \cdots, N-1$ remain unchanged while for $i = 1$ and $i = N$, they change as functions of λ. The gap for $i = 1$ and $i = N$ can be tuned to be equal to the value we need by tuning the corresponding nearest neighbor interactions $V_{i,i+1}$ since gap for link $i - i + 1$ is equal to $V_{i,i+1}\langle a_{i+1}a_i\rangle$. So both criteria are satisfied in the process of moving Majorana zero modes and at the same time we are able to calculate explicitly the many-body wave functions of the system. In Section A.3 and A.4, both criteria will be checked explicitly throughout the braiding process.

A.2 Non-Abelian transformation and gauge invariance

Consider a Hamiltonian $H(\lambda)$ depending continuously on λ with n degenerate levels which do not cross other levels. As $H(\lambda)$ is adiabatically varied and returned to the initial one, a set of n states which at time t_i are degenerate orthonormal eigenstates of $H(\lambda_i)$ undergo non-abelian transformation and each of the final states is a unitary transform of the initial states. For an arbitrary smooth set of bases $\psi_a(t)$, the solutions to the time dependent Schrodinger equations $\eta_a(t)$ can be written as

$$\eta_a(t) = U_{ab}(t)\psi_b(t) \tag{A.8}$$

with the initial condition $\eta_a(t_i) = \psi_a(t_i)$, $a = 1, 2, \cdots, n$. $U_{ab}(t)$ is found to be [62]

$$U(t) = P\exp\int_{t_i}^{t} A(\tau)d\tau, \tag{A.9}$$

where Berry connection A is given by

$$A_{ab} = (\psi_a, \dot{\psi}_b)^* \tag{A.10}$$

with $\dot{\psi}_b \equiv \partial \psi_b / \partial \tau$.

If we choose another set of basis $\tilde{\psi}(t) = \Omega(t)\psi(t)$, A transforms as

$$\tilde{A} = \dot{\Omega}\Omega^{-1} + \Omega A \Omega^{-1}, \tag{A.11}$$

and U transforms as

$$\tilde{U} = \Omega(t_i) U \Omega^{-1}(t). \tag{A.12}$$

The solutions to the time dependent Schrodinger equations $\tilde{\eta}_a(t)$ become

$$\tilde{\eta}_a(t) = \tilde{U}_{ab}(t)\tilde{\psi}_b(t) = \Omega_{ab}(t_i)\eta_b(t) \tag{A.13}$$

with initial condition $\tilde{\eta}_a(t_i) = \tilde{\psi}_a(t_i) = \Omega_{ab}(t_i)\psi_b(t_i)$. Equation (A.13) demonstrates gauge invariance of the evolution of the solutions, i.e., the evolution is independent of different choices of Ω so that the evolution of ground states is uniquely determined by their initial states (in equation A.13, the time evolution of $\tilde{\eta}_a(t)$ is independent of time dependence of $\Omega_{ab}(t)$ and is completely determined by the initial values $\Omega_{ab}(t_i)$). In the following two sections, we shall calculate evolution of degenerate ground states in different choices of bases to confirm the gauge independence and so to justify our choice of basis for calculating Berry phase in A.4.

A.3 Double interchange of zero Majorana fermions

In this and the next sections, we'll consider systems harboring four zero Majorana fermions γ_i, $i = 1, 2, 3, 4$ and interchange γ_1 and γ_2. It's simplest to discuss braiding in the diagonal basis: such a basis is given by $|00\rangle$ and $|11\rangle = f_1^\dagger f_2^\dagger |00\rangle$, $f_1 = \gamma_1 + i\gamma_2$ and $f_2 = \gamma_3 + i\gamma_4$ and we interchange positions of γ_1 and γ_2. In this basis, the off-diagonal Berry connections vanish by construction.

The off-diagonal Berry connection $\langle 00|\dot{11}\rangle$ ('$\cdot$' denotes derivative) is

$$\langle 00|\dot{11}\rangle = \langle 00|\dot{f}_1^\dagger f_2^\dagger|00\rangle + \langle 00|f_1^\dagger f_2^\dagger|\dot{00}\rangle = 0 \tag{A.14}$$

Both terms that contribute to $\langle 00|\dot{11}\rangle$ vanish: for the first term, we can first switch positions of $\dot{f}_1^\dagger$ and $f_2^\dagger$ with a minus sign since they anti-commute due to Fermi statistics and their exponentially small spatial overlap and next operate $f_2^\dagger$ on $\langle 00|$ giving zero by definition: $f_2|00\rangle = 0$; for the second term, $\langle 00|f_1^\dagger = 0$ by definition. In this basis, if we can make $|00\rangle$ and $|11\rangle$ real throughout the braiding, Berry phase vanishes for each state. Then braiding is completely determined by the explicit change (monodromy) of basis states. This can be realized in the set up shown in figure A.2. The arrows and links have the same meaning as discussed below equation A.7 in Section A.1. When a link goes from solid to dotted, it means the strength of the link decreases continuously to zero (and vice versa). An isolated dot denotes an unoccupied site. When the dot goes from isolated to connected by a link, the chemical potential on that site decreases to zero (and vice versa). According the rules given below equation A.7, one can easily read off the corresponding Hamiltonian for the process from figure A.2.

Adiabatic evolution of Hamiltonian according to figure A.2 yields double interchange of γ_1 and γ_2 at the end of the braiding and both of the operators continuously evolve back to themselves with extra minus sign (note that this result is the same as that with interchanging two vortices and therefore two MZMs twice in p+ip superfluids). Therefore $|11\rangle$ picks up an explicit phase of π relative to $|00\rangle$ at the end of the braiding. Combining with the (trivial) Berry phase contribution, the final states evolve to $|\eta(00)\rangle_f = e^{i\phi}|\eta(00)\rangle_i$, $|\eta(11)\rangle_f = e^{i(\phi+\pi)}|\eta(11)\rangle_i$ with initial condition $|\eta(00)\rangle_i = |00\rangle_i$ and $|\eta(11)\rangle_i = |11\rangle_i$ (we use η to denote actual solutions of time dependent Schrodinger equations). Now if we switch to another basis $|\tilde{00}\rangle = \alpha|00\rangle + \beta|11\rangle$ and $|\tilde{11}\rangle = \beta^*|00\rangle - \alpha^*|11\rangle$, with initial condition $|\eta(\tilde{00})\rangle_i = |\tilde{00}\rangle_i$ and $|\eta(\tilde{11})\rangle_i = |\tilde{11}\rangle_i$ (assume constant α and β), they should evolve to

$$\begin{aligned}|\eta(\tilde{00})\rangle_f &= \alpha|\eta(00)\rangle_f + \beta|\eta(11)\rangle_f = e^{i\phi}(\alpha|\eta(00)\rangle_i - \beta|\eta(11)\rangle_i)\\ |\eta(\tilde{11})\rangle_f &= \beta^*|\eta(00)\rangle_f - \alpha^*|\eta(11)\rangle_f = e^{i\phi}(\beta^*|\eta(00)\rangle_i + \alpha^*|\eta(11)\rangle_i).\end{aligned} \tag{A.15}$$

Each of them evolves into linear combination of the initial states. The U matrix in this basis should be identity according to equation (A.12) since the in the diagonal basis, U is identity. This can be easily verified. The Berry connection matrix elements are

$$\begin{aligned}
\langle \widetilde{00} | \dot{\widetilde{00}} \rangle &= 2\mathrm{Im}(\alpha^* \beta) \langle 00 | \dot{11} \rangle \\
\langle \widetilde{11} | \dot{\widetilde{11}} \rangle &= -\langle \widetilde{00} | \dot{\widetilde{00}} \rangle \\
\langle \widetilde{00} | \dot{\widetilde{11}} \rangle &= -\mathrm{Im}(\alpha^{*2} + \beta^{*2}) \langle 00 | \dot{11} \rangle,
\end{aligned} \tag{A.16}$$

which according to equation (A.14) all vanish.

So far, we have discussed particle non-conserving states. What about particle conserved states? Equation (A.14) is not strictly satisfied for finite size systems. In the thermodynamic limit, it is satisfied. The Berry phase associated with each basis state still vanishes since they are real after particle number projection. So in this braiding scheme, the braiding statistics is unchanged from particle non-conserving case.

To verify the above result, we have performed explicit calculations in the diagonal basis with average number of 4 electrons for particle non-conserving states (throughout the braiding, the hopping and gap parameter are set equal). Our calculations confirm that the two ground states evolve continuously as we expect. The two criteria listed in Section A.1 are satisfied and energy gap never closes during the braiding. There is one caveat: at the stage where the two Majorana fermions interchange places, the average particle number of $|11\rangle$ differs from that of $|00\rangle$ with maximum discrepancy of one electron in the middle of the stage. Although this issue is absent for some basis states, constant average particle number can not be satisfied for states in all bases. In practice, we may ensure the constant average particle number in one basis state and obtain the particle conserving state for the other basis state by applying particle number conserved BdG operators to the former state.

A.4 Single interchange of zero Majorana fermions

It's more interesting to know braiding statistics of interchanging two zero Majorana fermions once. This can be realized by T-junction proposed by Alicea et al [27]. It turns out that braiding in particle number conserved form can also realized in the same T-junction provided we can ensure constant average particle number by for example, moving the other two zero Majorana fermions. This can be achieved similarly to the double interchange scheme. The braiding process is shown in figure A.3. The arrows, links and isolated dots have the same meaning as discussed in the above section and the corresponding Hamiltonian can be easily read off from figure A.3 according to the rules laid out below equation A.7.

In the diagonal basis, the two basis functions are no longer real. In the particle non-conserved form, the two states have the same Berry phase during the interchange. However, it is not necessarily true for the particle conserved states. We may expect different braiding statistics for particle conserved states! Switching to another basis with real basis states doesn't alter the conclusion due to gauge invariance. Let us check gauge invariance by starting from a non-diagonal basis given by $|00\rangle$ and $|11\rangle = f_1^\dagger f_2^\dagger |00\rangle$ with $f_1 = \gamma_3 + i\gamma_1$ and $f_2 = \gamma_4 + i\gamma_2$. At the end of braiding, γ_1 becomes $\pm\gamma_2$ and γ_2 becomes $\mp\gamma_1$. We haven't specified the signs after the braiding which depend on braiding sequence (clockwise or counterclockwise). At the end of the braiding, the basis functions become

$$
\begin{aligned}
|00\rangle_f &= \frac{1}{\sqrt{2}}(|00\rangle_i \pm |11\rangle_i) \\
|11\rangle_f &= \frac{1}{\sqrt{2}}(|11\rangle_i \mp |00\rangle_i).
\end{aligned} \tag{A.17}
$$

The transformation matrix U for the solutions to the time dependent Schrodinger equations is found to be

$$
U = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{A.18}
$$

with $\theta = \int_{t_i}^{t_f} dt \langle 00(t)|\dot{11}(t)\rangle$. Combining equation (A.18) with (A.17), we get the solutions at the end of braiding

$$\begin{pmatrix} |\eta(00)\rangle_f \\ |\eta(11)\rangle_f \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 1 & \pm 1 \\ \mp 1 & 1 \end{pmatrix} \begin{pmatrix} |\eta(00)\rangle_i \\ |\eta(11)\rangle_i \end{pmatrix}$$
$$= \begin{pmatrix} \cos(\theta \pm \frac{\pi}{4}) & \sin(\theta \pm \frac{\pi}{4}) \\ -\sin(\theta \pm \frac{\pi}{4} & \cos(\theta \pm \frac{\pi}{4}) \end{pmatrix} \begin{pmatrix} |\eta(00)\rangle_i \\ |\eta(11)\rangle_i \end{pmatrix}. \tag{A.19}$$

Now, we switch back to the diagonal basis given by $|\tilde{00}\rangle$ and $|\tilde{11}\rangle = \tilde{f}_1^\dagger \tilde{f}_2^\dagger |\tilde{00}\rangle$ with $\tilde{f}_1 = \gamma_3 + i\gamma_4$ and $\tilde{f}_2 = \gamma_1 - i\gamma_2$. The diagonal basis states are related to the non-diagonal basis states by

$$|\tilde{00}\rangle = \frac{1}{\sqrt{2}}(|00\rangle - i|11\rangle)$$
$$|\tilde{11}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + i|11\rangle). \tag{A.20}$$

At the end of the braiding, they are

$$|\tilde{00}\rangle_f = e^{\pm i\pi/4}(|\tilde{00}\rangle_i$$
$$|\tilde{11}\rangle_f = e^{\mp i\pi/4}|\tilde{11}\rangle_i. \tag{A.21}$$

The U matrix is

$$U = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}. \tag{A.22}$$

From equation (A.20) and (A.19), we obtain the final solutions in the diagonal basis

$$
\begin{aligned}
\begin{pmatrix} |\eta(\tilde{00})\rangle_f \\ |\eta(\tilde{11})\rangle_f \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} |\eta(00)\rangle_f \\ |\eta(11)\rangle_f \end{pmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} \cos(\theta \pm \frac{\pi}{4}) & \sin(\theta \pm \frac{\pi}{4}) \\ -\sin(\theta \pm \frac{\pi}{4} & \cos(\theta \pm \frac{\pi}{4}) \end{pmatrix} \begin{pmatrix} |\eta(00)\rangle_i \\ |\eta(11)\rangle_i \end{pmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} \cos(\theta \pm \frac{\pi}{4}) & \sin(\theta \pm \frac{\pi}{4}) \\ -\sin(\theta \pm \frac{\pi}{4} & \cos(\theta \pm \frac{\pi}{4}) \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \begin{pmatrix} |\eta(\tilde{00})\rangle_i \\ |\eta(\tilde{11})\rangle_i \end{pmatrix} \\
&= \begin{pmatrix} e^{i(\theta \pm \frac{\pi}{4})} & 0 \\ 0 & e^{-i(\theta \pm \frac{\pi}{4})} \end{pmatrix} \begin{pmatrix} |\eta(\tilde{00})\rangle_i \\ |\eta(\tilde{11})\rangle_i \end{pmatrix}. \qquad \text{(A.23)}
\end{aligned}
$$

This is the same as obtained by combining equation (A.21) and (A.22)

$$
\begin{aligned}
\begin{pmatrix} |\eta(\tilde{00})\rangle_f \\ |\eta(\tilde{11})\rangle_f \end{pmatrix} &= \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} \begin{pmatrix} e^{\pm i\pi/4} & 0 \\ 0 & e^{\mp i\pi/4} \end{pmatrix} \begin{pmatrix} |\tilde{00}\rangle_i \\ |\tilde{11}\rangle_i \end{pmatrix} \\
&= \begin{pmatrix} e^{i(\theta \pm \frac{\pi}{4})} & 0 \\ 0 & e^{-i(\theta \pm \frac{\pi}{4})} \end{pmatrix} \begin{pmatrix} |\eta(\tilde{00})\rangle_i \\ |\eta(\tilde{11})\rangle_i \end{pmatrix}. \qquad \text{(A.24)}
\end{aligned}
$$

So consistency is satisfied. If θ is nonzero, then we get different braiding result for particle conserving states compared to particle non-conserving states where $\theta = 0$.

We have implemented calculations for eight lattice sites and on average four particles. Calculations are done in off-diagonal basis in which basis states are kept real during the interchange. Off-diagonal Berry phase θ (cf. matrix in equation A.18) are calculated. We found that for particle number conserving states with four particles, $\theta = 0$ consistent with result for particle number non-conserving states. Interestingly, $\theta = \pm 0.4$ for states in two and six particle number sectors respectively. It will be interesting to see how nonzero Berry phases away from average particle number scales with system size.

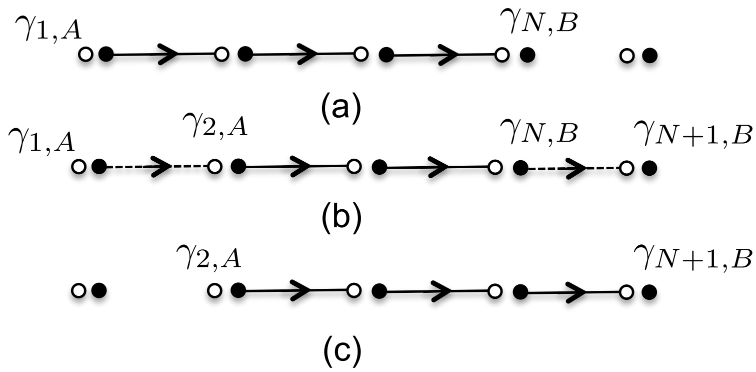

Figure A.1: Moving Majorana zero modes in a single wire. Black and white dots represent two Majorana fermions at each site. (a) initial configuration. (b) Moving both the left and right Majorana zero modes to the right by one site. (c) Final configuration.

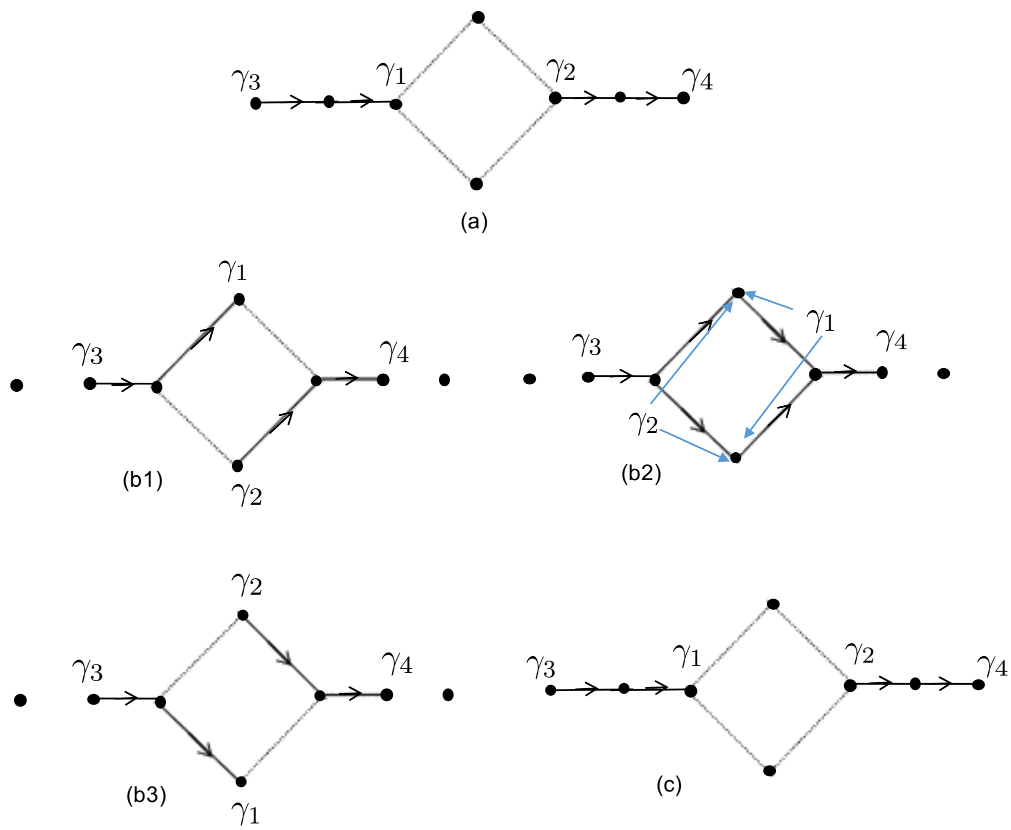

Figure A.2: Exchanging Majorana zero modes γ_1 and γ_2 twice in 1D Kitaev network. (a) Initial configuration. (b1) - (b3) Intermediate configuration. At (b2), γ_1 is localized at both top and bottom sites in the figure and so is γ_2; the former are localized on the right of the top and bottom sites (i.e., imaginary part of fermion, γ_B in the sense of figure A.1) and the latter are localized on the left (i.e., real part, γ_A). For simplicity, we didn't draw each site by two dots as we did in figure A.1. If we were to do that, then γ_1 is localized at the right dot on the top and bottom site and γ_2 is at the left dot on the top and the bottom site. The other two Majorana zero modes γ_3 and γ_4 are also moved, but they eventually go back to their initial positions and very importantly they never cross other Majorana zero modes. (c) Final configuration.

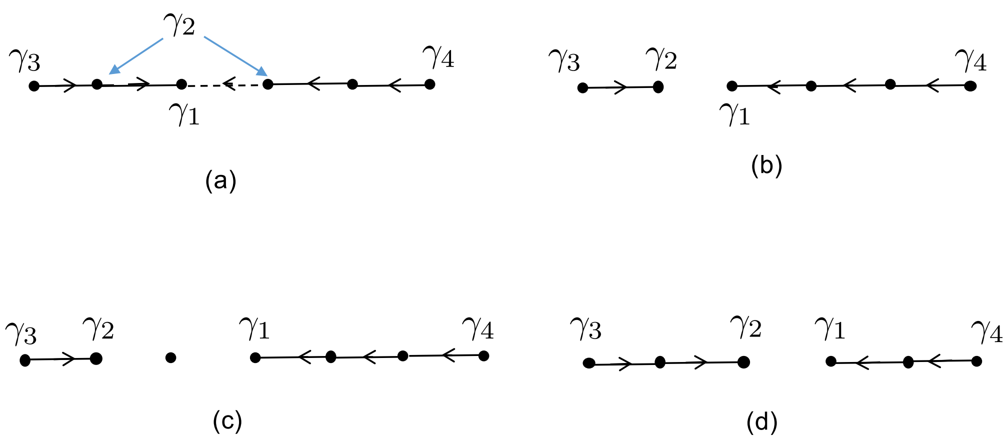

Figure A.3: Exchanging Majorana zero modes γ_1 and γ_2 in 1D Kitaev network. (a) γ_2 is moved to the left as indicated by the two blue arrows; in the process of moving, γ_2 is localized at two sites as pointed by the two blue arrows. (b) γ_1 and γ_2 are interchanged. (c) γ_1 is moved to the right to the original place of γ_2 before interchange. (d) γ_2 is moved to the right to the original place of γ_1 before interchange. The final configuration is the same as before interchange with γ_1 and γ_2 swapped places. From (b) to (c) and from (c) to (d), γ_4 is also moved to ensure particle number conservation.

Appendix B

Localized Quasiparticle in a Square Well Zeeman Trap

In this appendix, we derive energy spectrum of a localized quasiparticle in a square well Zeeman potential trap. For simplicity of notation, we'll present details at magnetic flux $\Phi = -1/2$, i.e., we'll solve equation 4.42. The corresponding result for general magnetic flux $\Phi = -1/2 + \lambda$ (corresponding to equation 4.43) will be listed without giving explicit derivation.

We solve equation 4.42 by expanding wave vector around p_F (we adopt linear momentum here, which is equivalent to angular momentum in 1D). Inside the well, i.e., between $\theta = 0$ and $\theta = \theta_L$, BdG quasiparticle states are plane waves; outside the well, they decay exponentially. We solve them by matching bound conditions at the edge of the well. It is convenient to write ratio of u and v as

$$\begin{aligned} \frac{v}{u} &= \frac{\triangle}{E + \Omega_o^{\pm}} = F_o^{\pm} \\ \frac{v}{u} &= \frac{\triangle}{E + V + \Omega_i^{\pm}} = F_i^{\pm}, \end{aligned} \tag{B.1}$$

where subscripts o and i refer to outside and inside the Zeeman trap respectively, I have omitted subscripts o, i and superscripts $\pm$ for u and v for notation simplicity. $\Omega_o^{\pm} = \pm\sqrt{\triangle^2 - E^2}i$, $\Omega_i^{\pm} = \pm\sqrt{(E+V)^2 - \triangle^2}$. Note that $\Omega_o^{\pm}$ is pure imaginary and this is the factor which gives rise to the exponential decay of the bound solutions outside the trap. Strictly speaking, there are eight boundary conditions, four of them coming from continuity conditions for u and v at the two trap edges, the other half coming from continuity conditions for the first derivatives of u and v. Since upon Andreev reflection, the momentum change is of order $\triangle/E_F$ compared to the Fermi momentum, the momenta of the particle and hole plane wave solutions differ only by order $\triangle/E_F$, relative to the Fermi momentum. If we ignore this small difference, the plane wave solutions for wave vectors in opposite directions become separate. We only need to match the continuity conditions for u and v (with wave vectors in one direction) and the continuity conditions for the first derivatives are automatically satisfied (this point is discussed by Demers and Griffin [63]). Within this approximation, the solutions with momentum in two opposite directions are degenerate, as is the case for the general gradually varying potential discussed in the main text. Consider a solution inside the trap of the form

$$\begin{aligned} u_i &= u_i^+ e^{ip_i^+\theta} + u_i^- e^{ip_i^-\theta} \\ v_i &= F_i^+ u_i^+ e^{ip_i^+\theta} + F_i^- u_i^- e^{ip_i^-\theta}, \end{aligned} \tag{B.2}$$

where $p_i^\pm = p_F + \frac{\Omega_i^\pm}{v_F}$; in getting the second equation, equation B.1 is used.

Similarly, the solution outside the trap is given by

$$\begin{aligned} u_o &= u_o^+ e^{ip_o^+(\theta-\theta_L)} + u_o^- e^{ip_o^-(2\pi-\theta)} \\ v_o &= F_o^+ u_o^+ e^{ip_o^+(\theta-\theta_L)} + F_o^- u_o^- e^{ip_o^-(2\pi-\theta)}, \end{aligned} \tag{B.3}$$

where $p_o^\pm = p_F + \frac{\Omega_o^\pm}{v_F}$.

Now by matching the boundary conditions at $\theta = 2\pi$ and $\theta = \theta_L$, we get the following equations at $\theta = 2\pi$

$$\begin{aligned} u_o^+ e^{ip_o^+(2\pi-\theta_L)} + u_o^- &= u_i^+ + u_i^- \\ F_o^+ u_o^+ e^{ip_o^+(2\pi-\theta_L)} + F_o^- u_o^- &= F_i^+ u_i^+ + F_i^- u_i^-. \end{aligned} \tag{B.4}$$

Similarly, the equations at $\theta = \theta_L$ are

$$\begin{aligned} u_o^+ + u_o^- e^{ip_o^-(\theta_L-2\pi)} &= u_i^+ e^{ip_i^+\theta_L} + u_i^- e^{ip_i^-\theta_L} \\ F_o^+ u_o^+ + F_o^- u_o^- e^{ip_o^-(\theta_L-2\pi)} &= F_i^+ u_i^+ e^{ip_i^+\theta_L} + F_i^- u_i^- e^{ip_i^-\theta_L}. \end{aligned} \tag{B.5}$$

Neglecting exponentially small terms in equation (B.4) and (B.5), we get the following equation

$$\frac{F_i^- - F_o^-}{F_o^- - F_i^+} = \frac{F_i^- - F_o^+}{F_o^+ - F_i^+} e^{i(p_i^- - p_i^+)\theta_L}. \tag{B.6}$$

This equation can be written as

$$\tan^{-1}\left(\frac{\sqrt{\triangle^2 - E^2}}{V - \sqrt{(E+V)^2 - \triangle^2}}\right) - \tan^{-1}\left(\frac{\sqrt{\triangle^2 - E^2}}{V + \sqrt{(E+V)^2 - \triangle^2}}\right) = -\frac{\sqrt{(E+V)^2 - \triangle^2}}{v_F}\theta_L + n\pi, \tag{B.7}$$

where n is integer.

We can find simple solutions to (B.7) in the limit of a wide trap, i.e., satisfying the condition

$$(E+V)^2 - \triangle^2 \ll V^2. \tag{B.8}$$

This condition is equivalent to

$$\begin{aligned} E + V - \triangle \sim \frac{v_F^2}{\triangle \theta_L^2} &\ll \frac{V^2}{\triangle} \\ \therefore \theta_L &\gg \theta_V, \end{aligned} \tag{B.9}$$

where $\theta_V = v_F/V$ is the length scale associated with the trap strength ($\hbar = 1$).

Under this condition, we can expand equation (B.7) to first order in $\sqrt{((E+V)^2 - \triangle^2)}/V$ and we get

$$\frac{1}{1 + \frac{\triangle^2 - E^2}{V^2}} = -\frac{\theta_L V}{2v_F} + \frac{n\pi}{2\sqrt{\frac{(E+V)^2 - \triangle^2}{V^2}}}. \tag{B.10}$$

Now, consider low bound states such that $(E + V - \triangle)/V \ll 1$ and $(\triangle - E)/V \sim 1$. Since the lhs of equation (B.10) is much smaller than 1 and the absolute values of both terms on the rhs of equation (B.10) are much greater than 1, we could set the lhs to zero. Hence, we arrive at the solution

$$E = \sqrt{(\frac{n\pi v_F}{\theta_L})^2 + \triangle^2} - V \tag{B.11}$$

This solution is consistent with the intuitive argument. For low bound states, all Zeeman energy V is saved since low bound wave functions are completely localized inside the trap, i.e., its range outside the trap is negligible, hence the term $-V$ in equation (B.11). The term $(2n\pi v_F/\theta_L)^2$ in the square root of the above equation is simply the kinetic energy of the quasiparticle since its momentum $\delta p = p - p_F$ is quantized by the trap as $2n\pi/(2\theta_L)$, with θ_L as the trap width.

It's interesting to compare this result with the spectrum for a quasiparticle trapped between two superconductors in a SNS junction [64]. There, we have a square well of the gap. Inside the well, the quasiparticle is in the superposition of normal particle and normal hole, and the effective quantization length is twice the trap width d due to Andreev reflection, so the spectrum is

$$E = \frac{2n\pi v_F}{2d} \tag{B.12}$$

Our result (B.11) is consistent with the standard picture that due to the Andreev reflection, the quantization length is twice the trap width.
The energy spectrum for general magnetic flux $\Phi = -1/2 + \lambda$ can be similarly found to be

$$(E+V)^2 - 4(E+V)p_F\lambda + 4p_F^2\lambda^2 = (\frac{2\pi n p_F}{\theta_L})^2 + \triangle^2 \tag{B.13}$$

Taking derivative with respect to λ, we obtain the result in the main text (cf. equation 4.44 in the absence of energy splitting), namely, near $\lambda = 0$, $dE/d\lambda = 2p_F$ (here p_F is angular momentum at Fermi energy with $\hbar = 1$, the energy unit is $\hbar^2/2mR^2$ with R radius of annulus).

Appendix C

Modified BdG Equations with Conserved Particle Number

We give here discussion on modified BdG equations taking into account particle number conservation. For this, when we evaluate quasiparticle energy as given by 5.22, we need to keep terms neglect in the mean-field approach and we get

$$
\begin{aligned}
\langle \alpha H \alpha^\dagger \rangle - \langle H \rangle &= \langle \alpha [H, \alpha^\dagger] \rangle + \langle \alpha \alpha^\dagger H \rangle - \langle H \rangle \\
&= \langle \{ \alpha, [H, \alpha^\dagger] \} \rangle - \langle [H, \alpha^\dagger] \alpha \rangle + \langle \alpha \alpha^\dagger H \rangle - \langle H \rangle. \qquad \text{(C.1)}
\end{aligned}
$$

The first term on the RHS is the dominant term, the second terms vanish provided α annihilates the $2N$-particle ground state, the last two terms cancel provided $\langle \alpha\alpha^\dagger \rangle = 1$: In order to satisfy the normalization condition $\langle \alpha\alpha^\dagger \rangle = 1$, we need to add a Lagrangian multiplier, so the expression we want to minimize is given by

$$
\langle \{ \alpha, [H, \alpha^\dagger] \} \rangle - \langle [H, \alpha^\dagger] \alpha \rangle + \langle \alpha \alpha^\dagger H \rangle - \langle H \rangle - \xi \langle \alpha \alpha^\dagger \rangle. \qquad \text{(C.2)}
$$

Once normalization condition is included through a Lagrangian multiplier, (C.2) can be simplified to

$$
\langle \{ \alpha, [H, \alpha^\dagger] \} \rangle - \langle [H, \alpha^\dagger] \alpha \rangle - \xi \langle \alpha \alpha^\dagger \rangle. \qquad \text{(C.3)}
$$

It is worth here emphasizing the importance of keeping terms involving α acting on the $2N$-particle ground state. This ensures that $E > 0$. This can be understood as follows. Imagine $\alpha^\dagger$ we found actually annihilates the ground state, i.e., $\alpha^\dagger$ is actually an annihilator. If we were to assume that α annihilate the ground state and discard the related terms, then we would get negative energy, corresponding to moving an excited state to the ground state by $\alpha^\dagger$. In general, we expect approximate qp eigenstate creation operator we found to be superposition of actual qp eigenstate creation operators and qp eigenstate annihilators with different eigenvalues. To get rid of the effect of these annihilators, we need to keep the terms containing α acting on the ground state.

Now, let's specify the Hamiltonian and the qp variational form. First consider a Zeeman trap applied to the superconducting system. The Hamiltonian is

$$H = \int dr \sum_\sigma \psi^\dagger(r) H_\sigma \psi_\sigma(r) - V_0 \int dr \psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r)\psi_\downarrow(r)\psi_\uparrow(r), \tag{C.4}$$

where $H_\sigma = H_0 - \sigma \cdot V_z$ with $\sigma = \pm 1$, V_z is Zeeman energy, H_0 is single particle kinetic energy. $-V_0 < 0$ is BCS contact interaction potential. The particle number conserving quasiparticle creation operator takes the following form

$$\alpha^\dagger = \int dr u(r)\psi_\uparrow^\dagger(r) + v(r)\psi_\downarrow(r)\Omega^\dagger, \tag{C.5}$$

where $\Omega^\dagger$ adds a pair of particles to the ground state.

Substituting (C.5) and (C.4) into $\langle\{\alpha, [H, \alpha^\dagger]\rangle$, we get

$$\begin{aligned}
\langle\{\alpha, [H, \alpha^\dagger]\}\rangle &= \int dr u^*(r) H_\uparrow u(r) - V_0 \int dr u^*(r) v(r) \langle \psi_\downarrow(r)\psi_\uparrow(r)\Omega^\dagger\rangle \\
&- \int dr v^*(r) H_\downarrow v(r) \langle \Omega\Omega^\dagger\rangle - V_0 \int dr u(r) v^*(r) \langle \Omega \psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r)\rangle \\
&+ W_{\text{pair}}.
\end{aligned} \tag{C.6}$$

The first four terms (neglecting Hartree-Fock terms) on the RHS is the standard expression corresponding to the generalized BdG energy taking into account the effect of pair operator on matrix elements. W_{pair} is the energy associated with the pair operator. It is given by

$$\begin{aligned}
W_{\text{pair}} &= \int dr|v(r)|^2\langle\Omega[H,\Omega^\dagger]\rangle + \int drH_\downarrow v(r)\int dr' u^*(r')\langle\psi_\downarrow(r)[\psi_\uparrow(r'),\Omega^\dagger]\rangle \\
&- \int drH_\uparrow u(r)\int dr' v^*(r')\langle[\Omega,\psi^\dagger_\uparrow(r)]\psi^\dagger_\downarrow(r')\rangle + \int drH_\downarrow v(r)\int dr' v^*(r')\langle\psi_\downarrow(r)[\Omega,\Omega^\dagger]\psi^\dagger_\downarrow(r')\rangle \\
&- \int drv(r)\int dr' u^*(r')\langle\psi_\downarrow(r)[\psi_\uparrow(r'),[H,\Omega^\dagger]]\rangle - \int drv(r)\int dr' v^*(r')\langle\psi_\downarrow(r)[\Omega,[H,\Omega^\dagger]]\psi^\dagger_\downarrow(r')\rangle \\
&- \int drv(r)\int dr' v^*(r')\langle\Omega\psi_\downarrow(r)[\psi^\dagger_\downarrow(r'),[H,\Omega^\dagger]]\rangle \\
&+ V_0\int drv(r)\int dr' u^*(r')\langle\psi^\dagger_\uparrow(r)\psi_\downarrow(r)\psi_\uparrow(r)[\psi_\uparrow(r'),\Omega^\dagger]\rangle \\
&+ V_0\int dru(r)\int dr' v^*(r')\langle[\Omega,\psi^\dagger_\uparrow(r)\psi^\dagger_\downarrow(r)]\psi_\downarrow(r)\psi^\dagger_\downarrow(r')\rangle \\
&+ V_0\int drv(r)\int dr' v^*(r')\langle[\Omega,\psi^\dagger_\uparrow(r)]\psi_\downarrow(r)\psi_\uparrow(r)\Omega^\dagger\psi^\dagger_\downarrow(r')\rangle \\
&+ V_0\int drv(r)\int dr' v^*(r')\langle\psi^\dagger_\uparrow(r)\psi_\downarrow(r)\psi_\uparrow(r)[\Omega,\Omega^\dagger]\psi^\dagger_\downarrow(r')\rangle.
\end{aligned} \tag{C.7}$$

Let's first consider the particle number conserved version of mean field BdG operators. $\Omega^\dagger$ acting on the $2N$-particle ground state generate $2N+2$-particle ground state, $u(r)$ and $v(r)$ are solutions to BdG particle non-conserving equations. Assume $\alpha^\dagger$ is normalized so that $\langle\alpha\alpha^\dagger\rangle = 1$. To order $1/N$, $\langle\Omega\Omega^\dagger\rangle = 1$. Assuming also zero point fluctuation of condensate doesn't appreciably change the order parameter from the mean field value, the first four terms on the RHS of (C.6) become the same as expression of the particle non-conserving BdG energy. Since the pair operator here is extensive, its commutation with local operator vanishes to order $1/N$ and $[\Omega,\Omega^\dagger]$ vanishes as well. So $W_{\text{pair}} = 2\mu\int dr|v(r)|^2$ since $[H,\Omega^\dagger] = 2\mu\Omega^\dagger$ to order $\triangle^2/\epsilon_F$. Thus we get

$$\begin{aligned}
\langle\{\alpha,[H,\alpha^\dagger]\}\rangle_{BdG} &= \int dru^*(r)H_\uparrow u(r) + \int dru^*(r)v(r)\triangle(r) \\
&- \int drv^*(r)(H_\downarrow - 2\mu)v(r) + \int dru(r)v^*(r)\triangle^*(r),
\end{aligned} \tag{C.8}$$

where gap is defined as $\triangle \equiv -V_0 < \psi_\downarrow(r)\psi_\uparrow(r) >$ in particle non-conserved form. Equation (C.8) gives mean field BdG qp energy.

It's attempting to optimize the extra Cooper pair $\Omega^\dagger$ by minimizing rhs of equation C.3. Aside from very complicated form of W_{pair} (equation C.7) which no longer takes the simple form as in the mean-field case due to possible localization of the Cooper pair, there is a much more serious problem which we have overlooked in the above consideration, the normalization of particle number. We have to ensure that the particle number after adding the quasiparticle is increase by 1. As we are dealing with many-body system, this will require the normalization of many-body state to be accurate to order $1/N^2$, which we don't know how to implement in practice (remember we also need to normalize $2N$-particle number conserved wave function which we don't know how to calculate with controlled accuracy either).

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